INFORMATION ONLY

WASTE ISOLATION PILOT PLANT
Sandia National Laboratories

Software Cover Sheet

Form Number: 461-B **Effective: 9/12/96**

Procedure: QAP 19-1 **Page** 1 **of** 1

1. Document Name: User's Manual
2. Document Version Number: 2.3
3. WPO Number: 43037
4. Software Name: FMT
5. Version ID: 2.3
6. Software Classification[1]: SNL - SW
7. Summary of Contents: COVER SHEET, DOCUMENT, REVIEW FORM, COMMENTS

   Total number of pages in body of document: 291

8. **Code Sponsor/Preparer(s) Signature(s)[2]:**

SANDRA C. BABB (Code Sponsor's Name *print*)	Sandra C. Babb (Signature)	5/13/97 (Date)
SANDRA C. BABB (Preparer's Name *print*)	Sandra C. Babb (Signature)	5/13/97 (Date)
CRAIG F. NOVAK (Preparer's Name *print*)	Craig F Novak (Signature)	13 May 97 (Date)

9. **Reviewer(s) Signature(s)[2]:**

YIFENG WANG (Reviewer's Name *print*)	Yifeng Wang (Signature)	5/13/97 (Date)
(Reviewer's Name *print*)	(Signature)	(Date)
(Reviewer's Name *print*)	(Signature)	(Date)

10. **Department Manager Approval:**

JOHN T. HOLMES (Department Manager's Name *print*)	John T. Holmes (Signature)	5/13/97 (Date)

11. **SCM Coordinator's Signature:**

JOHN J. LOUKOTA (SCM Coordinator's Name *print*)	John J. Loukota (Signature)	5/13/97 (Date)

(1) *Choose from classifications in Appendix A.*

(2) *If there are more than one preparer or reviewer, each person's responsibilities shall be delineated in the document. Each reviewer shall complete a reviewer's form which applies to the document reviewed, or document their review in a memorandum. The review documentation shall be included in the document. Attach additional Software Cover Sheets if there are more than three Code Sponsor/preparers or reviewers.*

WPO# 43037 Keywords: FMT, UM, , ,

SWCF File Code: SWCF- A (A or C WBS#) : 1.4.01.6.1 : QA : (Alpha Code (s)) :SFT

INFORMATION ONLY

User's Manual for FMT Version 2.3:

A Computer Code Employing the Pitzer Activity Coefficient Formalism for Calculating Thermodynamic Equilibrium in Geochemical Systems to High Electrolyte Concentrations

Sandra C. Babb and Craig F. Novak
Sandia National Laboratories

Document Version 2.3

WPO # 43037

January 9, 1997

Abstract

FMT is a FORTRAN computer code used to solve the systems of equations associated with the calculation of chemical equilibrium in geochemical systems at 25°C. FMT uses aqueous thermodynamics coupled with the Pitzer activity coefficient formalism to calculate equilibrium in highly concentrated electrolyte systems. The data base supplied with the code covers the chemical system Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-B-H_2O augmented to include Am(III), Pu(III), Nd(III), Th(IV), and Np(V). The data base is internally consistent and has provided reliable independent predictions of dissolved actinide concentrations under wide ranges of conditions.

Recent development of FMT has been sponsored by the Waste Isolation Pilot Plant (WIPP). This document is intended to serve two purposes: to provide an introduction on the capabilities and use of FMT, and to satisfy quality assurance requirements for the WIPP Project.

Acknowledgments

The preparation and development of this document was greatly facilitated by Scott Free, Dan Scott, and Yifeng Wang. Scott Free provided general chemistry support with equations and derivations for verifying hand calculations. Dan Scott coordinated editorial and word processing support. Yifeng Wang performed an extensive review of the code itself and verified the benchmarking calculations against data and other computer codes.

Table of Contents

1.0 INTRODUCTION 9
1.1 Software Identifier 11
1.2 Points of Contact 11
1.2.1 Code Sponsor 11
1.2.2 Code Consultant 11
2.0 FUNCTIONAL REQUIREMENTS 12
3.0 REQUIRED USER TRAINING AND/OR BACKGROUND 13
4.0 DESCRIPTION OF THE MODELS AND METHODS 14
4.1 Mathematical Model and Numerical Methods 14
4.2 The Pitzer Activity Coefficient Formalism 17
4.3 Inclusion of Pitzer Activity Coefficients 22
4.4 Charge Neutrality 23
4.5 Pseudoelements 24
5.0 CAPABILITIES AND LIMITATIONS OF THE SOFTWARE 25
6.0 USER INTERACTIONS WITH THE SOFTWARE 27
6.1 Overview 27
6.2 User-Supplied Input Files 28
6.3 Executing FMT 29
6.3.1 Organization of Files 29
6.3.2 DEC Environment with WIPP Computers 31
6.3.2.1 Fetching the Command File FMT_CUR.COM from CMS 31
6.3.2.2 Running FMT_CUR.COM 31
6.3.2.3 Examples 32
6.3.3 General DEC Environment 38
6.3.4 Macintosh Environment 38
6.4 Setting up and Running a Batch (Flash) Problem 39
6.4.1 Screen Display Descriptions 39
6.4.2 Using FOR088 File as INGUESS File 39
6.5 Setting up and Running a Titrate Problem 42
6.5.1 Using Volume Options (LOG10, LINEAR, and ASREAD) 42

6.5.2 Screen Display Descriptions 44
6.5.3 Titrate Sample Problem: Solubility Calculation 45
7.0 DESCRIPTION OF INPUT FILES 50
7.1 INPUT 51
7.1.1 Batch Problem 51
7.1.2 Titrate Problem 52
7.2 INGUESS 54
7.2.1 Batch Problem 54
7.2.2 Titrate Problem 57
7.3 Standard CHEMDAT Input File 58
7.3.1 CHEMDAT Data Flow 59
7.3.2 Data Sources for HMW_NP_AM_RTEST.CHEMDAT 59
7.3.3 Description of the HMW_NP_AM_RTEST.CHEMDAT File 61
7.3.4 Description of OUTPUT Listing of HMW_NP_AM_RTEST.CHEMDAT 66
7.4 Standard RHOMIN Input File 70
8.0 ERROR MESSAGES 72
8.1 Fatal Error Messages 74
8.1.1 Error: "Charge" abundance is not 74
8.1.2 Error: check problem type 75
8.1.3 Error: ERROR IN INITIAL ESTIMATE 75
8.1.4 Error: INPUT ERROR to 76
8.1.5 Error: MAXELEM= 'value for 76
8.1.6 Error: MAXSPEC= 'value for 76
8.1.7 Error: MUST PUT ALL AQUEOUS 77
8.1.8 Error: Negative Element or Species Abundance 77
8.1.9 Error: "NEW T" option 79
8.1.10 Error: No Convergence on Equi 79
8.1.11 Error: PROBLEM TOO LARGE FOR 79
8.1.12 Error: Species "H2O" must be first 80
8.1.13 Error: To use TITRATE option 80
8.1.14 Error: Trying to shift reaction 81

8.1.15 Error: VALID CHARGE BALANCE ELEMENT NOT 81
8.1.16 Error: Was expecting the "TITRATE" 81
8.2 System Error Messages.....82
8.3 Warning Messages.....82
8.3.1 Warning: BATCH CALCULATION ERRORS 82
8.3.2 Warning: CANNOT FIND LOCATION OF 83
8.3.3 Warning: "EXACT" mole amounts 83
8.3.4 Warning: MASS BALANCE ERRORS 84
8.4 Informational Messages.....84
8.4.1 AQ vio 'value of mu' 84
8.4.2 DONT HAVE ANY REACTIONS 84
8.4.3 MU(ttl)= 'value of mu' 85
8.4.4 SOLUBILITY PRODUCT VIOLATION 85
8.4.5 'count of ' Solubility Product Violations 85
8.4.6 Switching Routine Hung 86
9.0 DESCRIPTION OF OUTPUT FILES.....87
9.1 OUTPUT.....87
9.1.1 Batch Problem 87
9.1.2 Titrate Problem 92
9.2 FOR088.....95
9.3 TITRATE.....96
10.0 REFERENCES 98
11.0 APPENDICES 102
Appendix A: Sample Screen Display of BATCH_DOC.....103
Appendix B: Sample Screen Display of Np_NaCl_BM_LOG 105
Appendix C: Sample Screen Display of Np_NaCl_BM_LIN.....107
Appendix D: Sample Screen Display of Np_NaCl_BM 109
Appendix E: Sample Input File "BATCH_DOC.IN".....111
Appendix F: Sample Input File "Np_NaCl_BM_LOG.IN" 112
Appendix G: Sample Input File "Np_NaCl_BM_LIN.IN".....114
Appendix H: Sample Input File "Np_NaCl_BM.IN".....116

Appendix I: Listing of HMW_NP_AM_RTEST.CHEMDAT and References Cited in Listing 119

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT 128

Appendix K: Listing of HMW_NP_AM_RTEST.RHOMIN and References Cited in Listing 141

Appendix L: Sample Output File "BATCH_DOC.OUT" 142

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT" 144

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT" 161

Appendix O: Sample Output File "Np_NaCl_BM.OUT" 178

Appendix P: Sample Output File "BATCH_DOC.FOR088" 195

Appendix Q: Sample Output File "Np_NaCl_BM_LOG.TITRATE" 197

Appendix R: Sample Output File "Np_NaCl_BM_LIN.TITRATE" 200

Appendix S: Sample Output File "Np_NaCl_BM.TITRATE" 203

Appendix T: Command File FMT_CUR.COM 206

Appendix U: Derivation of CO_2 Fugacity 212

Appendix V: Memorandum on Current Release of Data Base 213

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np5_960823.CHEMDAT 232

Appendix X: Current Data Base, HMW.RHOMIN 280

Appendix Y: Review Forms 281

List of Figures

Figure 1. Input and Output Files for BATCH 28

Figure 2. Input and Output Files for TITRATE 28

Figure 3. Suggested data base organization. 30

Figure 4. Suggested input/output file organization 30

Figure 5. Titration problem using LINEAR option. 45

Figure 6. Calculated Total Np(V) and Np(V) Concentrations as a function of CO_3^{2-} concentration in 5.61 molal (5M) NaCl, and comparison with experimental measurements from Neck et al. (1994). 49

Figure 7. Batch INPUT file. 51

Figure 8. Titrate INPUT file. 53

Figure 9. Nassi-Schneiderman (N-S) chart showing FMT control flow. 60

List of Tables

Table 1. Example Np_CaCl_Bm_LOG.COM File for Running FMT in the DEC Environment 38

Table 2. Batch Problem Screen Display Description (See Appendix A for sample listing.) 40

Table 3. Titrate Options 43

Table 4. Titrate Problem Screen Display Description (See Appendices B, C, and D for sample screen displays of Np_NaCl_BM_LOG, Np_NaCl_BM_LIN, and Np_NaCl_BM, respectively.) 46

Table 5. INPUT File Parameters for Batch (See Appendix E for sample listing.) 52

Table 6. INPUT File Parameters for Titrate (See Appendices F, G, and H for sample listings of Np_NaCl_BM_LOG.IN, Np_NaCl_BM_LIN.IN, and Np_NaCl_BM.IN, respectively.) 55

Table 7. INGUESS File Parameters for Batch Problem 57

Table 8. INGUESS File Parameters for Titrate Problem 58

Table 9. Arbitrary Values Used for Standard Chemical Potentials 61

Table 10. CHEMDAT Input Parameters (Listing of HMW_NP_AM_RTEST.CHEMDAT provided in Appendix I.) 62

Table 11. OUTPUT File Description of CHEMDAT Input Parameters (See listing provided in Appendix J.) 66

Table 12. RHOMIN Input Parameters (See Appendix K for listing.) 71

Table 13. FMT Messages 72

Table 14. OUTPUT File Description for Batch (See Appendix L for sample listing.) 88

Table 15. OUTPUT File Description for Titrate (See Appendices M, N, and O for sample listings of Np_NaCl_BM_LOG.OUT, Np_NaCl_BM_LIN.OUT, and Np_NaCl_BM.OUT, respectively.) 93

Table 16. FOR088 File Description for Batch (See Appendix P for sample listing.) 96

Table 17. TITRATE File Description (Appendix Q) 96

1.0 INTRODUCTION

This User's Manual is intended to serve two purposes: to allow an interested user to learn what FMT does and to satisfy quality assurance requirements for the project that helped support the development of FMT. We have attempted to write this document so that persons not associated with the project can skip project-specific sections without skipping essential information about FMT.

The FMT program calculates chemical equilibrium in geochemical systems using aqueous thermodynamics and the Pitzer activity coefficient formalism (Pitzer, 1991). The name FMT derives from previous versions of the code used for fracture-matrix transport calculations, which are not supported in the release of FMT Version 2.3.

FMT computes the molal concentrations (moles of solute per kilogram of water solvent) of chemical species using the activity coefficient formalism of Pitzer (1991) as parameterized and reported for the sea water and evaporite system in Harvie et al. (1984) and Felmy and Weare (1986). For simplicity, this data base is referred to as the Harvie-Møller-Weare or HMW data base.

The Waste Isolation Pilot Plant (WIPP) application of the thermodynamic model involves predicting the solubility of actinides in the concentrated electrolyte solutions (brines) that occur at and around the WIPP site. To this end, the WIPP Project has measured the solubility and speciation behavior of several actinides in various oxidation states as a function of NaCl, $MgCl_2$, Na_2CO_3, $NaHCO_3$, K_2CO_3, KCl, and other more complex ionic systems. These data have been used to develop thermodynamic parameters consistent with those of the HMW data base. The FMT code is used by the WIPP Project to calculate actinide solubilities in concentrated electrolytes to support performance assessment of the WIPP.

The majority of the example problems in this User's Manual employ an early version of the thermodynamic data base that contained few actinide data. The actinide data base has been much expanded since this document was developed. Thus, the chemical calculations in the examples must be considered illustrative of FMT use only. Appendix V contains a memorandum documenting the most current release of the actinide thermodynamic data base with all data sources. Appendix W contains a listing of the most current release of the data base, called HMW_Am3Pu3Th4Np5_960823.CHEMDAT, and Appendix X contains a listing of the most current release of the data base, called HMW_Am3Pu3Th4Np5_960823.RHOMIN.

FMT calculates equilibrium on a closed system with fixed total element abundances. Water must be present and solid phases might or might not be present, depending on the particular chemical conditions. There are two modes of running FMT, one for single and one for multiple equilibrium problems. The single equilibrium problem, called a batch or flash problem, equilibrates one set of chemical abundances. The multiple equilibrium problem, called a titration problem, equilibrates two input solutions and then adds one solution to the other in user-specified volume increments to simulate a chemical titration.

FMT was intended to be used to support the WIPP performance assessment (PA) by generating tables of solubilities for actinides in the +III, +IV, +V, and +VI oxidation states, as a function of the relevant dominant variables influencing actinide solubilities in the WIPP system. These tables were to have been converted into equations to be used as input to the WIPP performance assessment codes, PANEL and NUTS, to provide a means of evaluating the solubility of actinides as a function of variables such as $CO_2(g)$ fugacity, hydrogen ion concentration, brine composition, and organic chelator concentrations.

This document serves as a User's Manual for FMT, as used to support the WIPP performance assessment calculations. As such, it describes the purpose and function of the code, user interaction with the code, and the equation and numerical methods employed by the code. Example of user-accessible input files, output files, and screen displays are appended to this manual.

1.1 Software Identifier

Code Name: FMT
WIPP Prefix: FMT_
Version Number: 2.3 04/01/97
Platforms: FORTRAN 77 for OpenVMS AXP, versions 6.1, on DEC Alpha;
Macintosh Power Book 5300CS,
Mac/OS 7.5.3 updated to Revision 2

1.2 Points of Contact

1.2.1 Code Sponsor

Sandra C. Babb
Sandia National Laboratories
Albuquerque, NM 87185-0660
Voice: (505) 844-7396 or (505) 848-0126
Fax: (505) 844-2018 or (505) 848-0881

1.2.2 Code Consultant

Craig F. Novak
Sandia National Laboratories
Albuquerque, NM 87185-1320
Voice: (505) 848-0619
Fax: (505) 848-0881

2.0 FUNCTIONAL REQUIREMENTS

R.1 FMT simulates solubility behavior of radionuclides in brines found in Castile, Rustler, and Salado Formations near the WIPP site.

R.2 FMT calculates chemical equilibrium using aqueous thermodynamics. It is based on the Harvie-Møller-Weare (HMW) data base augmented with radioactive elements.

R.3 FMT additionally mechanizes repetitive calculations, e.g., titrating a solution of one chemical composition with a solution of another chemical composition.

R.4 FMT supports calculations for highly charged aqueous species such as carbonate complexes with Americium (III), Thorium(IV), and Neptunium (V).

R.5 The "batch" simulation mode, also known as flash problems, calculates equilibrium abundances for one set of element abundances.

R.6 The "titrate" mode shall support explicit specification, i.e., adding user-specified volume for each titration increment.

R.7 The "titrate" mode shall support linear increments, i.e., adding a constant volume for each titration increment.

R.8 The "titrate" mode shall support logarithmic increments, i.e., adding a logarithmically increasing volume for each titration.

3.0 REQUIRED USER TRAINING AND/OR BACKGROUND

In order to run the FMT code successfully, the user will need a basic knowledge of

- Open VMS and Digital Equipment Co.'s (DEC's) Digital Command Language (DCL), if running the code on the DEC platform
- Power Macintosh 7100 operation, if running the code on a Macintosh platform.

To interpret the results of FMT, a chemistry background is required. A user should have a

- BS in Chemistry, or the equivalent
- experience in evaluating the plausibility of solid phases with respect to the particular chemical system
- sound understanding of chemical reaction equilibrium analysis.

To understand how the FMT code works and the theory and algorithms upon which FMT is based, the user should also have a basic understanding of

- thermodynamics
- partial derivatives
- linear algebra (through senior undergraduate level)
- numerical methods (graduate or senior level undergraduate level).

4.0 DESCRIPTION OF THE MODELS AND METHODS

4.1 Mathematical Model and Numerical Methods

FMT solves chemical equilibrium problems, as defined by linear material balance equations and nonlinear reaction equilibrium equations as given in standard chemical thermodynamics texts such as Denbigh (1981) and Smith and Van Ness (1975). An extensive survey of numerical methods developed specifically to solve these problems is given in Smith and Missen (1991). In particular, FMT uses the "Villars-Cruise-Smith" (VCS) algorithm, which is explained in Section 6.4.4 of Smith and Missen (1991). A brief overview of the VCS algorithm, as presented in Smith and Missen (1991) follows. Interested readers are referred to Smith and Missen (1991) for a more detailed discussion.

If the Gibbs free-energy function G is viewed as a function of the reaction-extent variables $\bar{\xi}$, then the chemical equilibrium problem is that of minimizing $G(\bar{\xi})$; i.e.,

$$\frac{\partial G}{\partial \bar{\xi}} = \mathbf{0} \tag{1}$$

Equation 1 is equivalent to the classical chemical formulation of the equilibrium conditions

$$\Delta \mathbf{G} \equiv \mathbf{N}^{\mathrm{T}} \bar{\mu}\left(\bar{\xi}\right) = 0\,, \tag{2}$$

where

$\mathbf{N}^{\mathrm{T}}$ = the complete, transposed stoichiometric matrix: the $(N \times R)$ matrix whose columns are the R stoichiometric vectors; that is, $\mathbf{N} = (\bar{\nu}_1, \bar{\nu}_2, \ldots, \bar{\nu}_R)$; entry (j) of $\mathbf{N}$ is ν_{ij}, and

$\bar{\mu}$ = chemical-potential vector with entries μ_i.

A first-order algorithm approach for minimizing $G(\bar{\xi})$ requires that the variables $\bar{\xi}$ be adjusted at each iteration by amounts $\delta\bar{\xi}$:

$$\begin{aligned} \delta\xi_j^{(m)} &= -\left(\frac{\partial G}{\partial \xi_j}\right)^{(m)} = -\Delta G_j^{(m)} \\ &= -\sum_{i=1}^{N'} \nu_{ij}\, \mu_i^{(m)}; \qquad\qquad j = 1,2,\ldots R, \end{aligned} \tag{3}$$

where

m = iteration index,

ν_{ij} = stoichiometric coefficient of species i in stoichiometric vector (equation) j,

N' = number of species excluding inert species,

μ_i = chemical potential of species i, and

R = maximum number of linearly independent chemical equations.

The mole numbers are adjusted by means of

$$\delta n_i^{(m)} = \sum_{j=1}^{R} \nu_{ij} \delta \xi_j^{(m)}; \quad i=1,2,...N', \tag{4}$$

where n_i = the number of moles of species i.

As with first-order optimization methods in general, this algorithm has been found to converge rather slowly, and therefore is not widely used.

In a second-order algorithm approach for minimizing $G(\bar{\xi})$, the Newton-Raphson method can be applied to Equation 2, which yields

$$\delta \bar{\xi}^{(m)} = -\left(\frac{\partial^2 G}{\partial \bar{\xi}^2}\right)^{-1}_{\mathbf{n}^{(m)}} \left(\frac{\partial G}{\partial \bar{\xi}}\right)_{\mathbf{n}^{(m)}}, \tag{5}$$

where $\mathbf{n}$ = species-abundance vector with entries n_i. This approach requires the solution of a set of $R = (N' - M)$ linear equations on each iteration (where M is the number of elements). Because N' is usually large compared with M, the numerical solution of these linear equations can be very time consuming and this approach is not widely used.

The VCS algorithm, an intermediate between the above first- and second-order methods, provides a way to reduce the computational effort involved in the solution of the linear equations.

The VCS algorithm begins with Equation 5, the Hessian matrix ($\partial^2 G/\partial \vec{\xi}^2$) for which, in the case of a single ideal phase, can be expressed as

$$\frac{\partial^2 G}{\partial \xi_i \partial \xi_j} = \frac{\partial}{\partial \xi_j}\left(\sum_{k=1}^{N'} \nu_{ki}\mu_k\right)$$

$$= RT\sum_{k=1}^{N'}\sum_{l=1}^{N'} \nu_{ki}\nu_{lj}\left(\frac{\delta_{kl}}{n_k} - \frac{1}{n_t}\right); \qquad j = 1,2,\ldots R\ , \tag{6}$$

where

R = the gas constant, 8.3143 J mole^{-1} K^{-1},

T = absolute temperature (K)

δ_{kl} = the Kronecker delta function; $\delta_{kl} = 1$, if $k = l$; $\delta_{kl} = 0$, if $k \neq l$,

n_k = number of moles of species k, and

n_t = total number of moles.

Smith and Missen (1991) explain in Section 6.4.4 how the Hessian matrix in Equation 6 can be expressed as

$$RT\left(\frac{\partial^2 G}{\partial \xi_i \partial \xi_j}\right)^{-1} \approx \left(\frac{1}{n_{i+M}} + \sum_{k=1}^{M}\frac{\nu_{ki}^2}{n_k} - \frac{\bar{\nu}_i^2}{n_t}\right)^{-1}\delta_{ij}\ , \tag{7}$$

where $\bar{\nu}_i$ is the sum of the stoichiometric coefficients in stoichiometric equation i; i.e. $\bar{\nu}_i = \sum_{k=1}^{N'} \nu_{ki}$

The VCS algorithm for a single ideal phase uses Equation 5 with Equation 7 and iteratively adjusts each stoichiometric equation by an amount

$$\delta\xi_j^{(m)} = -\left(\frac{1}{n_{j+M}^{(m)}} + \sum_{k=1}^{M}\frac{\nu_{kj}^2}{n_k^{(m)}} - \frac{\bar{\nu}_j^2}{n_t}\right)^{-1}\frac{\Delta G_j^{(m)}}{RT}; \qquad j = 1,2,\ldots R. \tag{8}$$

As is explained in Section 4.4, FMT replaces one of the R element balances in Equation 8 with the charge balance, which not only specifies the material balance of the "replaced" element but also constrains the solution to be charge neutral. The charge balance can be shown to be a linear combination of the individual material balances.

The thermodynamics of concentrated electrolyte solutions (brines) requires consideration of the chemical nonidealities of the system. FMT uses the activity coefficient model of Pitzer (1991) and the internally consistent data base described by Harvie et al. (1984) and Felmy and Weare (1986) as the basis for modeling chemical nonidealities. These references provide extensive detail about the version of the Pitzer activity coefficient formalism used in FMT. A brief discussion of the Pitzer activity coefficient model follows in Section 4.2.

4.2 The Pitzer Activity Coefficient Formalism

The Pitzer activity coefficient formalism is a set of mathematical equations for calculating activity coefficients for aqueous species, and is valid from dilute systems through the concentrated brines observed at the WIPP Site. The theoretical and historical development of this formalism can be traced though Pitzer (1991), and references therein.

The implementation of the Pitzer activity coefficient formalism within FMT is based on the forms of the equations as presented in Harvie and Weare (1980), Harvie et al. (1984), and Felmy and Weare (1986). Because there is no difference in the mathematical formulation from these references and FMT, only the equations in Felmy and Weare (1986) are presented below. The interested reader will find a comprehensive presentation of these equations in the three cited publications.

The activities of the species a_i can be defined by the following equation:

$$\left(\frac{\partial G}{\partial n_i}\right)_{T,P,n} \equiv \mu_i = \mu_i^0 + RT \ln a_i , \qquad \text{(A.1a*)}$$

where μ_i^0 = the standard chemical potential for species i. Activity is defined for each solute species i by

* Equation numbering scheme in Felmy and Weare (1986) is duplicated for this discussion.

$$a_i = \gamma_i m_i \tag{A.1b}$$

and, for the solvent, by

$$\ln a_{H_2O} = \frac{-W}{1000}\left(\sum_i m_i\right)\phi \tag{A.1c}$$

where

γ_i = the activity coefficient of the solute species,

m_i = the molality of the solute species,

W = the molecular weight of water,

$\sum_i m_i$ = the sum over all solutes (cations, anions, and neutral species), and

ϕ = the osmotic coefficient.

While the chemical potentials for pure phases (e.g., minerals) are constant at fixed temperature and pressure, the fugacity of gas-phase species, f_i, is defined as follows:

$$\frac{\mu_i}{RT} = \frac{\mu_i^0}{RT} + \ln(f_i) . \tag{A.1d}$$

The remaining variables lacking explicit definition are the excess functions γ_i and $(\phi - 1)$. These functions, rewritten below, are modeled using the semiempirical equations of Pitzer (1973) and co-workers. (Note that, in the Pitzer equations presented below, I = ionic strength, and that subscripts *M*, *X*, and *N* refer to cations, anions, and neutrals, respectively. The remaining terms are explained following the presentation of the Pitzer equations.)

$$(\phi-1)\frac{\left(\sum_i m_i\right)}{2} = -\frac{A^{\phi} I^{3/2}}{1+bI^{1/2}} + \sum_c \sum_a m_c m_a (B^{\phi}_{ca} + ZC_{ca}) + \sum_c \sum_{c'>c} m_c m_{c'} \left(\Phi^{\phi}_{cc'} + \sum_a m_a \psi_{cc'a}\right)$$

$$+ \sum_a \sum_{a'>a} m_a m_{a'} \left(\Phi^{\phi}_{aa'} + \sum_c m_c \psi_{aa'c}\right) + \sum_n \sum_c m_n m_c \lambda_{nc}$$

$$+ \sum_n \sum_a m_n m_a \lambda_{na} + \sum_n \sum_c \sum_a m_n m_c m_a \zeta_{nca} \qquad \text{(A.2a)}$$

$$\ln\gamma_M = z_M^2 F + \sum_a m_a (2B_{Ma} + ZC_{Ma}) + \sum_c m_c \left(2\Phi_{Mc} + \sum_a m_a \psi_{Mca}\right)$$

$$+ \sum_a \sum_{a'>a} m_a m_{a'} \psi_{aa'M} + |z_M| \sum_c \sum_a m_c m_a C_{ca} + \sum_n m_n (2\lambda_{nM}) + \sum_n \sum_a m_n m_a \zeta_{naM} \qquad \text{(A.2b)}$$

$$\ln\gamma_X = z_M^2 F + \sum_c m_c (2B_{Xc} + ZC_{Xc}) + \sum_a m_a \left(2\Phi_{Xa} + \sum_c m_c \psi_{Xca}\right)$$

$$+ \sum_c \sum_{c'>c} m_c m_{c'} \psi_{cc'X} + |z_X| \sum_c \sum_a m_c m_a C_{ca} + \sum_n m_n (2\lambda_{nX}) + \sum_n \sum_c m_n m_c \zeta_{ncX} \qquad \text{(A.2c)}$$

$$\ln\gamma_N = \sum_c m_c (2\lambda_{Nc}) + \sum_a m_a (2\lambda_{Na}) + \sum_c \sum_a m_c m_a \zeta_{Nca} \qquad \text{(A.2d)}$$

$$F = -A^{\phi}\left(\frac{I^{1/2}}{1+bI^{1/2}} + \frac{2}{b} ln\left(1+bI^{1/2}\right)\right) + \sum_c \sum_a m_c m_a B'_{ca}$$

$$+ \sum_c \sum_{c'>c} m_c m_{c'} \Phi'_{cc'} \sum_a \sum_{a'>a} m_a m_{a'} \Phi'_{aa'} \qquad \text{(A.2e)}$$

$$C_{MX} = \frac{C^{\phi}_{MX}}{2|Z_M Z_X|^{1/2}} \tag{2b}$$

$$Z = \sum_i |z_i| m_i \tag{2c}$$

A^{ϕ} is one third of the Debye-Hückel limiting slope (A in the following empirical equation):

$$\ln\gamma_i^{DH} = -\frac{A\sqrt{I}}{1 + Ba_i\sqrt{I}} + \dot{B}_i I,$$

as presented on page 981 of Harvie and Weare [1980].) Here A^{ϕ} equals 0.39 at 25°C. The second virial coefficients, B, are given the following ionic strength dependence:

$$B^{\phi}_{MX} = \beta^{(0)}_{MX} + \beta^{(1)}_{MX} e^{-\alpha_1\sqrt{I}} + \beta^{(2)}_{MX} e^{-\alpha_2\sqrt{I}} \tag{3a}$$

$$B_{MX} = \beta^{(0)}_{MX} + \beta^{(1)}_{MX} g\left(\alpha_1\sqrt{I}\right) + \beta^{(2)}_{MX} g\left(\alpha_2\sqrt{I}\right) \tag{3b}$$

$$B'_{MX} = \beta^{(1)}_{MX} \frac{g'\left(\alpha_1\sqrt{I}\right)}{I} + \beta^{(2)}_{MX} \frac{g'\left(\alpha_2\sqrt{I}\right)}{I} \tag{3c}$$

The functions g and g' are defined by

$$g(x) = 2\frac{\left(1 - (1+x)e^{-x}\right)}{x^2} \tag{4a}$$

$$g'(x) = -2\frac{\left(1-\left(1+x+\frac{x^2}{2}\right)e^{-x}\right)}{x^2} \tag{4b}$$

with $x = \alpha_1\sqrt{I}$ or $= \alpha_2\sqrt{I}$. When either cation M or anion X is univalent, $\alpha_1 = 2.0$ and $\alpha_2 = 12$. For 2 - 2 pairs, $\alpha_1 = 1.4$ and $\alpha_2 = 12$. For all electrolyes, $b = 1.2$. For 2 - 3 and higher pairs, $\alpha_1 = 1.4$ and $\alpha_2 = 50$. The dimensions of α_1 and α_2 are $kg^{½}mole^{-½}$. The virial coefficients, Φ, which depend upon ionic strength, are given the following form:

$$\Phi^{\phi}_{ij} = \theta_{ij} + {}^{E}\theta_{ij}(I) + I\,{}^{E}\theta'_{ij}(I) \tag{5a}$$

$$\Phi_{ij} = \theta_{ij} + {}^{E}\theta_{ij}(I) \tag{5b}$$

$$\Phi'_{ij} = {}^{E}\theta'_{ij}(I) \tag{5c}$$

The functions ${}^{E}\theta_{ij}(I)$ and ${}^{E}\theta'_{ij}(I)$ are functions only of ionic strength and the electrolyte pair type.

The activity coefficient parameters, λ_{ni} and ζ_{nij}, representing the interactions between neutral species and ions, are taken to be constant. The third virial coefficients, C^{ϕ}_{MX} and Ψ_{ijk}, are also assumed to be independent of ionic strength.

The complete set of parameters defining the model for nonideal behavior of electrolyte solutions are as follows:

- $\beta^{(0)}_{MX}$, $\beta^{(1)}_{MX}$, $\beta^{(2)}_{MX}$, and C^{ϕ}_{MX} for each cation-anion pair
- θ_{ij} for each cation-cation and anion-anion pair
- Ψ_{ijk} for each cation-cation-anion and anion-anion-cation triplet

- λ_{ni} and ζ_{nij} for ion-neutral and ion-ion-neutral interactions.

Many of these parameters can be assigned a value of zero. The above parameters are tabulated in the CHEMDAT data base (Section 7.3.3, Appendices I and J).

4.3 Inclusion of Pitzer Activity Coefficients

The activity coefficients are included within FMT according to the "Indirect Methods Based on Algorithms for Ideal Systems" documented in Section 7.3.1 of Smith and Missen (1991). A brief overview of the discussion provided in Section 7.3.1 of Smith and Missen (1991) follows.

The following is an expression for the chemical potential:

$$\mu_i(T,P,\mathbf{x}) = \mu_i^*(T,P) + RT\ln\gamma_i(T,P,\mathbf{x})x_i\,, \tag{9}$$

and

$$\lim_{x_i\to 1}\gamma_i = 1 \qquad \text{(Raoult convention)}$$

or

$$\lim_{x_i\to 0}\gamma_i = 1 \qquad \text{(Henry convention)}$$

where

$\mathbf{x}$ = mole-fraction vector with entries x_i,

T = temperature,

P = pressure, and

μ_i^* = standard chemical potential of species i.

Equation 9 may be rewritten as

$$\mu_i = \mu_i^* + RT\ln\gamma_i(T,P,\mathbf{n}) + RT\ln x_i\,, \tag{10}$$

where $\mathbf{n}$ = species-abundance vector with entries n_i.

When the first two terms on the right-hand side of Equation 10 are combined, the equation can be formally rewritten as

$$\mu_i = \mu_i^*[T, P, \mathbf{n}^*, (T, P)] + RT \ln x_i \tag{11}$$

where μ_i^* is now a function of T and P through the unknown equilibrium solution $\mathbf{n}^*$.

The calculation procedure is iterative, in which the first step is to compute the equilibrium composition assuming ideality ($\gamma_i = 1$), yielding a first approximation to the system mole numbers $\mathbf{n}^{(1)}$. Then the activity coefficients $\bar{\gamma}$ for the nonideal system are computed from a known chemical potential expression at the $\mathbf{n}^{(1)}$ composition. In the next step, the equilibrium composition in the "ideal" system is computed from Equation 11, with μ_i^* replaced by

$$\mu_i^{*(1)} = \mu_i^* + RT \ln \gamma_i(T, P, \mathbf{n}^{(1)}). \tag{12}$$

This process is repeated until the composition on successive iterations remains constant to within some specified tolerance. FMT uses this procedure in conjunction with the VCS algorithm described in Section 4.1.

4.4 Charge Neutrality

Charge neutrality is maintained within FMT in order to represent the charge neutral state of aqueous solutions that occurs in the laboratory and the environment. It has been shown (see for example Smith and Missen, 1991) that a linear combination of the element material balances produces the charge balance equation. Note that, because of the methods computers use to store numbers, it is extremely unlikely that the computed solution will have a charge equal to zero. Rather, the total charge will be a small number within some tolerance from zero, i.e., within the range -ltoll < computed charge < +ltoll. The rootfinding tolerance generally used within FMT is 10^{-6} (specified in the CHEMDAT file), indicating that the computed charge would be within the range -10^{-6} < computed charge < 10^{-6}. In practice, the computer charge is always much closer to zero; usually the absolute value of the computed charge is in the range 10^{-12} to 10^{-18}. It is unimportant whether the total charge is positive or negative so long as it is approximately zero. FMT replaces one of the element balances with the charge balance, which both specifies the material balance on the "replaced" element and constrains the solution to be charge neutral. The

element to be replaced with the charge balance, FORTRAN variable RPLWCHG, can be any element, but is usually set to Oxygen because it will be present in all aqueous chemical systems. FMT cannot calculate a charge imbalanced solution composition. However, should one wish to specify a charge imbalance, fictitious aqueous species "PosIon+" and "NegIon-" can be used to do so. For example, entering a concentration of "PosIon+" at 0.1 m will cause the solution to have a net negative charge of 0.1 m.

4.5 Pseudoelements

Pseudoelement is the name given to mathematical constructs that are not actual chemical elements but mathematically are treated the same as an element. Some of the pseudoelements used within FMT in the past have been "Electron:EL", "PosIon:EL", "NegIon:EL", "ClO4:EL", and "Charge:EL". Perchlorate, ClO_4, is a pseudoelement because it is a combination of elements treated as an element. That is, the unit "ClO4:EL" cannot be divided into its constituent elements during simulations with FMT. Organic ligands are treated as pseudoelements, including "Oxalate:EL", "Citrate:EL", "Acetate:EL", "Lactate:EL", and "EDTA:EL". This prevents these moieties from undergoing chemical reactions that alter the organic species, while allowing the organic ligands to complex with protons and other aqueous species. In contrast, although sulfur always occurs with 4 oxygen atoms in the data base, SO_4 is not treated as a pseudoelement, although it could have been.

5.0 CAPABILITIES AND LIMITATIONS OF THE SOFTWARE

FMT calculates chemical equilibrium for user-specified total element amounts for aqueous or aqueous + mineral geochemical systems. All chemical elements specified by the user must be included in the data base used by FMT in order for calculations to proceed correctly. The original FMT data base file used to develop this document, HMW_NP_AM_RTEST.CHEMDAT (described in Section 7.3), is limited to the elements H, O, Na, K, Mg, Ca, Cl, S, B, C, Br, and P, and the pseudoelements "Am(III)," "Np(V)," "ClO_4," "PosIon", "NegIon", and "Charge." (Element names contained in quotes are not strictly chemical elements, but they are called pseudoelements because they are treated mathematically as indivisible units, and thus behave numerically as though they were chemical elements.) The species that can be formed from these elements, aqueous and solid, are only those that are included in the data base. The HMW_NP_AM_RTEST data base is listed in Appendix I; the most current data base release, HMW_Am3Pu3Th4Np5_960823, is documented in Appendix V and listed in Appendix W. The user is responsible for determining whether the data base included in FMT is appropriate for his/her chemical system.

It is important to note that FMT does not model gas phases explicitly. However, the effects of chemical equilibrium between a solution and a gas phase with constant fugacities for all soluble gas phase constituents can be modeled by creating hypothetical but thermodynamically viable solid phases in the solution. The standard chemical potentials of these fictitious solids are calculated from the constant gas fugacities.

Several scenarios for WIPP disposal rooms suggest there will be CO_2 gas present. It is therefore desirable to calculate the effects of CO_2 gas on the aqueous and solid chemistry in the disposal room, and in turn on dissolved actinide concentrations. While FMT cannot explicitly model the gas phase, it can model a system with constant CO_2 gas fugacity by proper declaration of a CO_2 solid phase, as discussed below.

Thermodynamics allows the declaration of a hypothetical CO_2 "solid" phase to mimic the effects of constant CO_2 gas fugacity:

$$CO_2(g) \leftrightarrow CO_2(\text{"solid"}) \tag{13}$$

At equilibrium, this reaction is described by the relationship

$$\frac{\mu^0_{CO_2(\text{"solid"})}}{RT} = \frac{\mu^0_{CO_2(g)}}{RT} + \ln f_{CO_2}, \tag{14}$$

where f_{CO_2} is the $CO_2(g)$ fugacity, which can be thought of as an effective partial pressure for $CO_2(g)$. Equation 14, which makes use of the standard convention that the activity of a pure solid phase is unity, allows one to simulate a system with a constant $CO_2(g)$ fugacity as long as the CO_2 "solid" phase is present. See Novak (1995k) for details.

Other particular items to note are listed below:

- Oxidation-reduction (redox) reactions are not supported in any of the data bases.
- The "Am(III)" and "Np(V)" models in HMW_NP_AM_RTEST.CHEMDAT data base are preliminary and provisional, and were updated in the HMW_AM3Pu3Th4Np5_960823.CHEMDAT data base. Additional updated versions of the CHEMDAT data base for use with FMT will be issued as they are developed.
- The radioactive elements uranium(IV), uranium(VI) and other elements may be added in future versions of the FMT data base. These additions will be modifications to the data base only (CHEMDAT) and will not require code changes.

6.0 USER INTERACTIONS WITH THE SOFTWARE

6.1 Overview

FMT requires three input data files—INPUT, INGUESS, and CHEMDAT. An additional input file RHOMIN is required for titration problems. In the INPUT file the user sets the problem parameters and specifies the solution composition by providing the *total element* abundances. Alternatively, the user could specify the same solution composition by setting the *species* abundances in the INGUESS file. The CHEMDAT file is a data base that contains species names, characteristics, and Pitzer parameters. RHOMIN, another data base file, contains mineral densities. FMT input files are discussed in detail in Section 7.0.

Note that "abundance" means the total amount, an extrinsic quantity, e.g., 3 moles of Na, 2 moles of Cl, 1 mole of Br. The intrinsic quantity, commonly moles per kg H_2O within FMT, is calculated based on the extrinsic amount of water that can be formed from the specified element abundances. This is the technical definition for the abundance entries. In practice, it is convenient to specify about 1 kg of water (about 55.5 moles of O and 111.0 moles of H) to allow the abundances in the INPUT and INGUESS files to be looked at on a molal (or approximately, molar) basis. (A convenient way to put all species concentrations in the INGUESS file on a nearly exact molal basis is through use of the FOR088 output file, which contains a column of species concentrations that have been normalized to a 1 kg H_2O basis. These concentrations can be copied to an INGUESS file to put all species in the INGUESS file on a molal basis, although technically it is still the extrinsic species abundances that are given. This merely "normalizes" all extrinsic abundances to a "per kg H_2O" basis.)

*****WARNING*****
The user should not and is not expected to change the CHEMDAT and RHOMIN files that are provided with the FMT code when using FMT in support of the WIPP.

FMT generates a primary file OUTPUT and a secondary file, depending on the problem. FOR088 is the secondary file for batch problems, while TITRATE is the secondary file for titrate problems. Both the FOR088 and TITRATE files are subsets of their respective OUTPUT files, reordered by chemical species for user convenience. Because the format of FOR088 is the same as that of INGUESS, FOR088 output can be modified and renamed as the INGUESS file to build increasingly complex chemical systems. Output files are discussed in detail in Section 9.0.

Figures 1 and 2 illustrate the input and output files for batch and titrate problems, respectively. The input files labeled as static are the data base files.

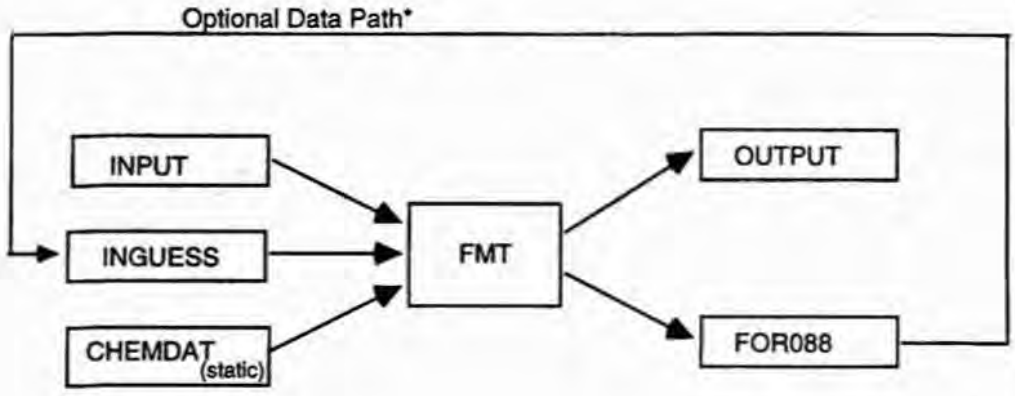


Figure 1. Input and Output Files for BATCH

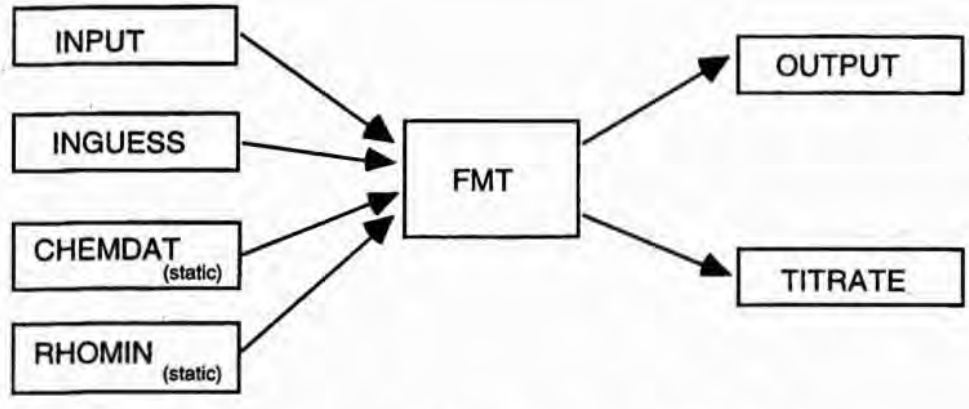


Figure 2. Input and Output Files for TITRATE

6.2 User-Supplied Input Files

The user creates and modifies parameters in the INPUT and INGUESS files using a convenient editor. After specifying a title for identifying the problem (usually naming the solution composition) and setting character flags in the INPUT file, the user enters the elemental

amounts required for a specific solution. The user must specify the amounts of all elements in the same order as the elements are listed in the CHEMDAT file.

The INGUESS file, if FMT is instructed to read it, provides total abundances of each element through the assignment of the total amount for each species in the CHEMDAT file. All amounts must be specified as total abundances, i.e., number of moles in the (unspecified) control volume. The user must state the moles for each species in the same order as the species are listed in the CHEMDAT file, starting with H_2O. FMT adds the species amounts with the appropriate stoichiometric coefficients to get to the total element abundances, and converts these extrinsic quantities to molality using the mass of water that can be formed from the given solution composition.

FMT reads the entire INPUT file. If the character strings 'MOLES' and 'EXACT' are set in the INPUT file, then FMT reads the moles for each species from the INGUESS file and calculates the molal amounts of all the elements. If 'nMOLES' and 'nEXACT' strings are set, then FMT uses the elemental mole amounts as stated in the INPUT file. In this case, the INGUESS file must exist although it may be an empty file, i.e., a file containing no data.

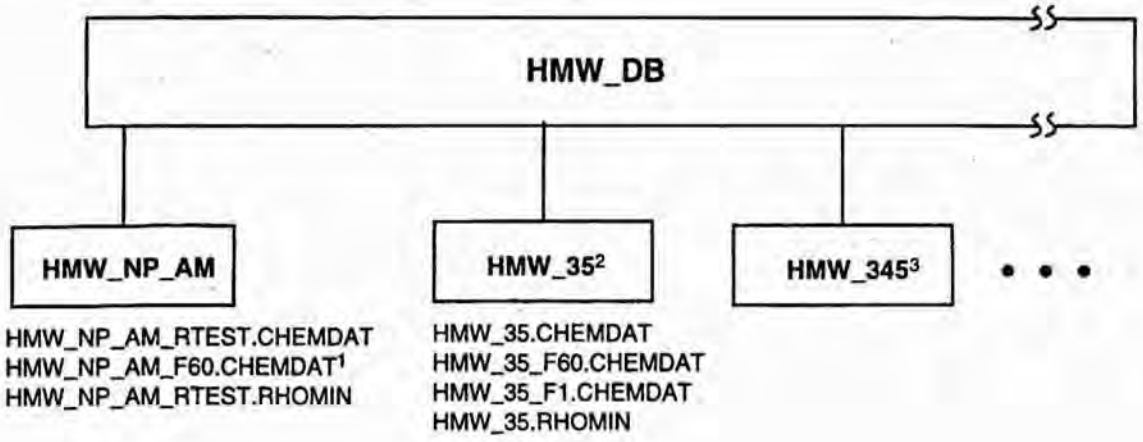
6.3 Executing FMT

6.3.1 Organization of Files

A suggested method for organizing folders or directories while running FMT on the DEC Alpha, Macintosh, or PC platforms is shown in Figures 3 and 4. Using this approach, the user groups

- all data base files (CHEMDAT and RHOMIN) in one folder. Beneath a major folder labeled "HMW_DB," Figure 3 shows two subfolders, labeled "HMW_NP_AM" and "HMW_35," which each contain unique CHEMDAT and RHOMIN data base files.

- the IN and INGUESS files in another folder. Beneath a major folder labeled "Test Cases," Figure 4 shows two problem-labeled folders, "BATCH_DOC" and "NP_NACL_BM," which each contain separate sets of input files. The "BATCH_DOC" input files are located under each version number folder.



Notes
1. Same as HMW_NP_AM_RTEST.CHEMDAT, except a declaration of CO_2 "solid" fugacity = 60.0 atm was added.
2. Contains updates on thermodynamic parameter values and complexation data for Np(V) and Np(V); F1 and F60 designate modifications to CHEMDAT file to reflect CO_2 "solid" fugacity at 1 and 60 atm.
3. Folder for future CHEMDAT data bases for Actinides in III, IV, V oxidation states.

Figure 3. Suggested data base organization.

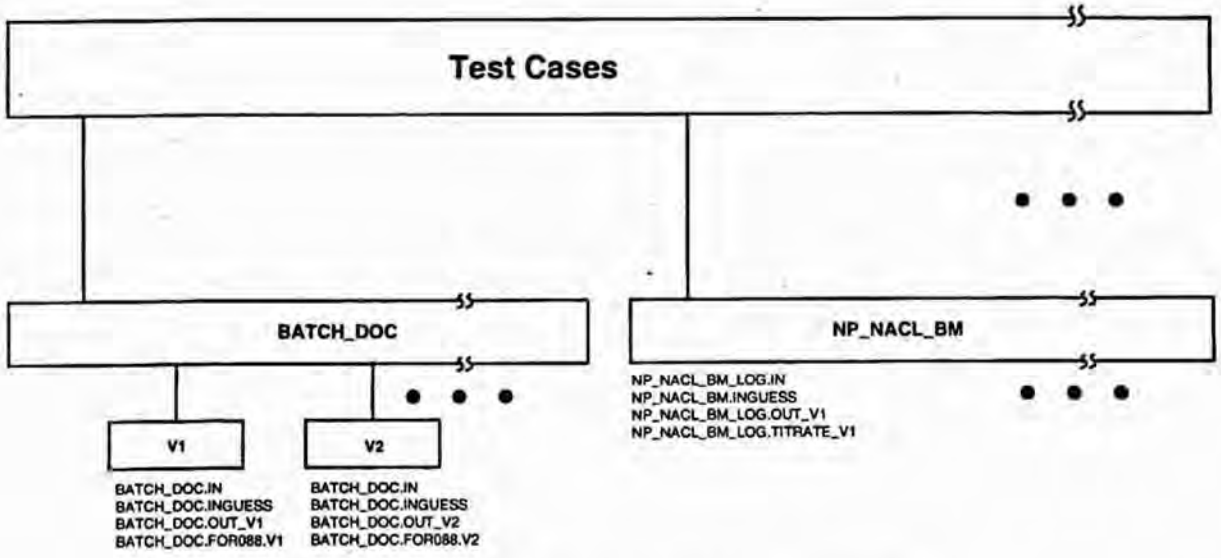


Figure 4. Suggested input/output file organization.

- the ouput files in either the same problem-labeled folder or another folder (beneath the problem-labeled folder) labeled with version numbers "V1," "V2," and so on. Both options are shown in Figure 4.

6.3.2 DEC Environment with WIPP Computers

The user can use the command file FMT_CUR.COM to run FMT on the Sandia NWER network with Digital's Alpha machine BEATLE. This file is located in the FMT library. All files in the library are under control of Digital's Configuration Management System (CMS). This library contains FMT data base files, source code and command files. The user can retrieve the command file FMT_CUR.COM from the FMT library using the CMS "fetch" command. For ease in executing FMT, the command file should be in the same directory where the input files reside.

6.3.2.1 Fetching the Command File FMT_CUR.COM from CMS

To retrieve the command file FMT_CUR.COM, the user logs into BEATLE and types in the symbol "nonpa_cms_syms" to define other CMS symbols, and the command "libfmt" to specify the FMT library. Then the user locates the directory/subdirectory where his/her input files reside by typing in a "set default (sd)" command. The command "cfe fmt_CUR.com" copies the command file into the user's current directory. The lines are:

```
$nonpa_cms_syms
$libfmt
$sd [username.user_inputfile_directory]
$cfe fmt_960823.com
```

The command file can be copied from directory to directory. The user does not need to fetch the file each time. FMT_CUR.COM also issues the lines "nonpa_cms_syms" and "libfmt" so the user does not need to type those two lines for each login.

6.3.2.2 Running FMT_CUR.COM

To execute "@FMT_CUR" the user must always be logged into BEATLE. The user should be in the directory that contains the .IN and .INGUESS files before starting FMT_CUR. To execute the command the user types in:

```
$@FMT_CUR
```

The user will be prompted to supply a **substring** for the CHEMDAT and RHOMIN files, the input file's name, and whether the Pitzer parameters should be echoed in the file. To retrieve a list of all CHEMDAT and RHOMIN files, the user can simply type in "FMT" since all data base files are prefixed with the "FMT_HMW_" string. Any substring of the data base file name can be typed in if the user knows the partial name or the date, such as 960823. The input file name must not contain the extensions (".IN" or ".INGUESS") and it must be the same for both the IN and INGUESS files.

After listing the CHEMDAT files that match the substring specified, the user is prompted to select a CHEMDAT file. The user can select a file by either double clicking on the file name, copying the file name and pasting it to the waiting request, or typing the entire name. Then a listing of all RHOMIN files matching the substring is displayed and the user is prompted to select a RHOMIN file.

Finally, the user is asked if FMT should echo the data base in the OUTPUT file. The CHEMDAT data bases can contain an enormous amount of data, which the user may not want to include the OUTPUT file.

*****WARNING*****

The FMT_CUR command deletes all chemdat and rhomin files with the "FMT_" prefix from the user's current directory before fetching any CHEMDAT or RHOMIN file.

6.3.2.3 Examples

The following examples show what (in boldface) a user types in response to a "$" prompt line or FMT's request. All other lines are BEATLE's operating system response, CMS's response, or FMT's response. FMT_CUR.COM generates the log file with the time and date stamp in the file's name. The log file records the explicit information on the build of the most current executable "FMT_PA97" and the complete input and output file names used in the runs.

Example #1 - Running the batch problem BATCH_DOC

The input file names and extensions for the BATCH_DOC problem are BATCH_DOC.IN and BATCH_DOC.INGUESS. Referring to the directory listing (dir) before and after the run, the program FMT generated the files BATCH_DOC.OUT and BATCH_DOC.FOR088. CMS fetched the files FMT_HMW_NP_AM_RTEST.CHEMDAT and FMT_HMW_NP_AM_RTEST.RHOMIN. A listing of the terminal session follows:

```
$ @fmt_cur
Enter chemdat file name to search on: np_am
Enter rhomin file name to search on: np_am
Enter input file name (without .extension): batch_doc
%CMS-I-LIBIS, library is WP$NONPA_CMSROOT:[FMT]
%CMS-S-LIBSET, library set
-CMS-I-SUPERSEDE, library list superseded

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.CHEMDAT "Initial load"
FMT_HMW_NP_AM_960823.CHEMDAT "CHEMDAT DATA BASE FILE FOR FMT 2.2 REGRESSION
TESTING"
FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
FMT_HMW_NP_AM_RTEST.CHEMDAT "CHEMDAT DATA BASE FILE FOR FMT 2.3 REGRESSION
TESTING"
Select CHEMDAT name from list above: FMT_HMW_NP_AM_RTEST.CHEMDAT
Your CMS library list consists of:
   WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element
WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.RHOMIN "Initial load"
FMT_HMW_NP_AM_960823.RHOMIN "RHOMIN DATA BASE FILE FOR FMT 2.2 REGRESSION
TESTING"
FMT_HMW_NP_AM_RTEST.RHOMIN "RHOMIN DATA BASE FILE FOR FMT 2.3 REGRESSION
TESTING"
Select RHOMIN name from list above: FMT_HMW_NP_AM_RTEST.RHOMIN
Your CMS library list consists of:
   WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element
WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.RHOMIN fetched
Enter "Y" or "y" to echo data base in OUT file: y

                image name: "FMT_PA97"
                image file identification: "P PA97 2.3"
                image file build identification: ""
                link date/time:  1-APR-1997 09:55:34.40
                linker identification: "A11-14"

DG_BYPASS flag set to nDG_BYPASS
[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs
FMT V2.3
DATA BASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

Accuracy of reactions is                1.0000E-06
Minimum elemental abundance is          1.0000E-18
Number of Aqueous Species is              50

ACTIVITY COEF. FLAG PITZACT
Finished do 10:  read b(0) b(1) b(2) cphi
Finished do 20:  read theta(c,c)
Finished do 30:  read theta(a,a)
Finished do 40:  read psi(c,c,a)
Finished do 50:  read psi(a,a,c)
Finished do 55:  read neucat(n,c)
Finished do 65:  read neuani(n,a)
Finished do 66:  read ptztsi(n,c,a)
using PITZER ACTIVITY COEFFICIENT model
```

```
Charge Balance replaces element Oxygen

Char Flags: FLOW/BATCH/TITRATE:  BATCH      UNUSED
this is a BATCH problem

Echo of Mole Specifications:  nMOLES     nEXACT
ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH
  110.222364000000      Hydrogen
  55.1654821000000      Oxygen
 0.200000000000000      Sodium
 1.000000000000000E-002 Potassium
 1.000000000000000E-003 Magnesium
 1.000000000000000E-004 Calcium
 0.110000000000000      Chlorine
 1.000000000000000E-003 Sulfur
 1.000000000000000E-004 Carbon
 0.000000000000000E+000 PosIon
 0.000000000000000E+000 NegIon
 0.000000000000000E+000 Air
 1.000000000000000E-007 Boron
 0.000000000000000E+000 Bromine
 0.000000000000000E+000 TracerEl
 0.000000000000000E+000 Th(IV)
 0.000000000000000E+000 Am(III)
 0.000000000000000E+000 U(VI)
 0.000000000000000E+000 Np(V)
 0.000000000000000E+000 ClO4-(EL)
 0.000000000000000E+000 Phosphorus
 0.000000000000000E+000 Electron
 4.906053920000000E-017 Charge
.LT. (MINABU*1.d-6) moles NaBO2.NaCl.2H2O___Teepleite_(20_C); del&switch
.LT. (MINABU*1.d-6) moles NaB5O8.5H2O_____Sodium_Pentaborate; del&switch
.LT. (MINABU*1.d-6) moles NaOH(aq).....to.titrate.base.only; del&switch
.LT. (MINABU*1.d-6) moles HCl(aq).......to.titrate.acid.only; del&switch
.LT. (MINABU*1.d-6) moles K2B4O7.4H2O___K-Tetraborate_(30_C); del&reopt
.LT. (MINABU*1.d-6) moles B4O5(OH)4=                B4O5(OH)4=; del&reopt
.LT. (MINABU*1.d-6) moles K8H6(SO4)7_________________Misenite; del&reopt
.LT. (MINABU*1.d-6) moles K8H4(CO3)6.3H2O___K-Sequicarbonate; del&switch
.LT. (MINABU*1.d-6) moles B3O3(OH)4-              B3O3(OH)4-; del&switch
.LT. (MINABU*1.d-6) moles Ca4Cl2(OH)6.13H2O__CaOxychloride A; del&switch

************SOLUBILITY PRODUCT VIOLATION*************
** Mg(OH)2_____________________Brucite **  1.00E+01 **

************SOLUBILITY PRODUCT VIOLATION*************
** Mg2Cl(OH)3.4H2O______MgOxychloride **  6.69E+00 **

         2 Solubility Product Violations
Adding solid Mg(OH)2_____________________Brucite
.LT. (MINABU*1.d-6) moles NaOH(aq).....to.titrate.base.only; del&switch
.LT. (MINABU*1.d-6) moles HCl(aq).......to.titrate.acid.only; del&switch
.LT. (MINABU*1.d-6) moles B4O5(OH)4=                B4O5(OH)4=; del&switch
.LT. (MINABU*1.d-6) moles B3O3(OH)4-              B3O3(OH)4-; del&switch
pH (-log[aH+]); pmH(-log[mH+])      12.8532      12.7140
fCO2(g); log[fCO2(g)]=                                    6.983E-13    -12.2
Total Diagonal Inversions          84
Total Stoichiometric Reoptimizations               9
SINGLE BATCH EQUILIBRATION COMPLETED
$ dir

Directory U1:[SCBABB.FMT.UM]

BATCH_DOC.FOR088;1  BATCH_DOC.IN;1      BATCH_DOC.INGUESS;1 BATCH_DOC.OUT;1
```

```
BATCH_DOC_APR29_0941.LOG;1                FMT_CUR.COM;1
FMT_HMW_NP_AM_RTEST.CHEMDAT;1
FMT_HMW_NP_AM_RTEST.RHOMIN;1

Total of 8 files.
```

FMT_CUR.COM recorded the screen output in the file BATCH_DOC_APR29_0941.LOG. A listing of the log file follows:

```
$ type batch_doc_apr29_0941.log
   "INPUT" = "BATCH_DOC.IN" (LNM$PROCESS_TABLE)
   "INGUESS" = "BATCH_DOC.INGUESS" (LNM$PROCESS_TABLE)
   "CHEMDAT" = "FMT_HMW_NP_AM_RTEST.CHEMDAT" (LNM$PROCESS_TABLE)
   "RHOMIN" = "FMT_HMW_NP_AM_RTEST.RHOMIN" (LNM$PROCESS_TABLE)
   "OUTPUT" = "BATCH_DOC.OUT" (LNM$PROCESS_TABLE)
   "FOR088" = "BATCH_DOC.FOR088" (LNM$PROCESS_TABLE)
   "TITRATE" = "BATCH_DOC.TITRATE" (LNM$PROCESS_TABLE)

               image name: "FMT_PA97"
               image file identification:  "P PA97 2.3"
               image file build idenficiation: " "
               link date/time:  1-APR-1997 09:55:34.40
               linker identification: "A11-14"

$
```

Example #2 - Running the titrate problem NP_NACL_BM

For a titrate problem such as NP_NACL_BM, the input files are NP_NACL_BM.IN and NP_NACL_BM.INGUESS. FMT generates NP_NACL_BM.OUT, and NP_NACL_BM.TITRATE.

```
$ dir

Directory U1:[SCBABB.FMT.UM]

FMT_CUR.COM;1       NP_NACL_BM.IN;1     NP_NACL_BM.INGUESS;1

Total of 3 files.
$ @fmt_cur
Enter chemdat file name to search on: np_am
Enter rhomin file name to search on: np_am
Enter input file name (without .extension): np_nacl_bm
%CMS-I-LIBIS, library is WP$NONPA_CMSROOT:[FMT]
%CMS-S-LIBSET, library set
-CMS-I-SUPERSEDE, library list superseded

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.CHEMDAT "Initial load"
FMT_HMW_NP_AM_960823.CHEMDAT "CHEMDAT DATA BASE FILE FOR FMT 2.2 REGRESSION
TESTING"
FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
FMT_HMW_NP_AM_RTEST.CHEMDAT "CHEMDAT DATA BASE FILE FOR FMT 2.3 REGRESSION
TESTING"
Select CHEMDAT name from list above: FMT_HMW_NP_AM_RTEST.CHEMDAT
```

```
Your CMS library list consists of:
   WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element
WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.RHOMIN "Initial load"
FMT_HMW_NP_AM_960823.RHOMIN "RHOMIN DATA BASE FILE FOR FMT 2.2 REGRESSION
TESTING"
FMT_HMW_NP_AM_RTEST.RHOMIN "RHOMIN DATA BASE FILE FOR FMT 2.3 REGRESSION
TESTING"
Select RHOMIN name from list above: FMT_HMW_NP_AM_RTEST.RHOMIN
Your CMS library list consists of:
   WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element
WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.RHOMIN fetched
Enter "Y" or "y" to echo data base in OUT file: n

                image name: "FMT_PA97"
                image file identification: "P PA97 2.3"
                image file build identification: ""
                link date/time:  1-APR-1997 09:55:34.40
                linker identification: "A11-14"

DG_BYPASS flag set to nDG_BYPASS
Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl
FMT V2.3
DATA BASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

Accuracy of reactions is                1.0000E-06
Minimum elemental abundance is          1.0000E-18
Number of Aqueous Species is              50

ACTIVITY COEF. FLAG PITZACT
PITZER Data Base NOT Echoed in this Run
Finished do 10:  read b(0) b(1) b(2) cphi
Finished do 20:  read theta(c,c)
Finished do 30:  read theta(a,a)
Finished do 40:  read psi(c,c,a)
Finished do 50:  read psi(a,a,c)
Finished do 55:  read neucat(n,c)
Finished do 65:  read neuani(n,a)
Finished do 66:  read ptztsi(n,c,a)
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

Char Flags: FLOW/BATCH/TITRATE:  TITRATE    EXPLICIT
this is a TITRATION problem

Character Flags:  J.C. nMOLES      nEXACT
Character Flags:  I.C. nMOLES      nEXACT
pH (-log[aH+]); pmH(-log[mH+])      11.7497       11.6199
fCO2(g); log[fCO2(g)]=                                    2.171E-07    -6.66
pH (-log[aH+]); pmH(-log[mH+])       5.3205        5.9141
fCO2(g); log[fCO2(g)]=                                    3.400E-02    -1.47
TITRATION Character Flags
  cdum1= TITRATE       cdum2= ASREAD
reading titrant volumes from input file
  First Volume Added =          0.10 mL
  Final Volume Added =         10.00 mL
```

```
pH (-log[aH+]); pmH(-log[mH+])      5.3205      5.9141
fCO2(g); log[fCO2(g)]=                                    3.400E-02    -1.47
pH (-log[aH+]); pmH(-log[mH+])      5.6451      6.2386
fCO2(g); log[fCO2(g)]=                                    2.716E-02    -1.57
pH (-log[aH+]); pmH(-log[mH+])      5.9936      6.5870
fCO2(g); log[fCO2(g)]=                                    1.847E-02    -1.73
pH (-log[aH+]); pmH(-log[mH+])      6.2353      6.8286
fCO2(g); log[fCO2(g)]=                                    1.290E-02    -1.89
pH (-log[aH+]); pmH(-log[mH+])      6.6996      7.2930
fCO2(g); log[fCO2(g)]=                                    5.484E-03    -2.26
pH (-log[aH+]); pmH(-log[mH+])      7.9427      8.5359
fCO2(g); log[fCO2(g)]=                                    3.555E-04    -3.45
pH (-log[aH+]); pmH(-log[mH+])      8.3317      8.9250
fCO2(g); log[fCO2(g)]=                                    1.461E-04    -3.84
pH (-log[aH+]); pmH(-log[mH+])      8.5655      9.1587
fCO2(g); log[fCO2(g)]=                                    8.559E-05    -4.07
pH (-log[aH+]); pmH(-log[mH+])      8.7166      9.3098
fCO2(g); log[fCO2(g)]=                                    6.060E-05    -4.22
pH (-log[aH+]); pmH(-log[mH+])      8.8722      9.4653
fCO2(g); log[fCO2(g)]=                                    4.250E-05    -4.37
pH (-log[aH+]); pmH(-log[mH+])      9.2225      9.8154
fCO2(g); log[fCO2(g)]=                                    1.922E-05    -4.72
pH (-log[aH+]); pmH(-log[mH+])      9.4695     10.0620
fCO2(g); log[fCO2(g)]=                                    1.108E-05    -4.96
pH (-log[aH+]); pmH(-log[mH+])      9.8493     10.4406
fCO2(g); log[fCO2(g)]=                                    4.873E-06    -5.31
pH (-log[aH+]); pmH(-log[mH+])     10.2955     10.8825
fCO2(g); log[fCO2(g)]=                                    2.019E-06    -5.69
pH (-log[aH+]); pmH(-log[mH+])     10.6594     11.2341
fCO2(g); log[fCO2(g)]=                                    1.106E-06    -5.96
End of AutoTitration Problem
$ dir

Directory U1:[SCBABB.FMT.UM]

FMT_CUR.COM;1        FMT_HMW_NP_AM_RTEST.CHEMDAT;1
FMT_HMW_NP_AM_RTEST.RHOMIN;1
NP_NACL_BM.IN;1      NP_NACL_BM.INGUESS;1                    NP_NACL_BM.OUT;1
NP_NACL_BM.TITRATE;1                    NP_NACL_BM_APR29_1122.LOG;1

Total of 8 files.
$ type np_nacl_bm_apr29_1122.log
   "INPUT" = "NP_NACL_BM.IN" (LNM$PROCESS_TABLE)
   "INGUESS" = "NP_NACL_BM.INGUESS" (LNM$PROCESS_TABLE)
   "CHEMDAT" = "FMT_HMW_NP_AM_RTEST.CHEMDAT" (LNM$PROCESS_TABLE)
   "RHOMIN" = "FMT_HMW_NP_AM_RTEST.RHOMIN" (LNM$PROCESS_TABLE)
   "OUTPUT" = "NP_NACL_BM.OUT" (LNM$PROCESS_TABLE)
   "FOR088" = "NP_NACL_BM.FOR088" (LNM$PROCESS_TABLE)
   "TITRATE" = "NP_NACL_BM.TITRATE" (LNM$PROCESS_TABLE)

                image name: "FMT_PA97"
                image file identification: "P PA97 2.3"
                image file build identification: ""
                link date/time:  1-APR-1997 09:55:34.40
                linker identification: "A11-14"

Pitzer Data Base NOT echoed in this Run
```

6.3.3 General DEC Environment

A suggested method for running FMT under a general DEC environment is given in Table 1 using the file structure of Figures 3 and 4. The command file is written assuming the executable, (here called FMT2P3.EXE to reflect that it is version 2.3) is in FMT.DIR, the parent directory to NP_NACL_BM.DIR.

Table 1. Example Np_CaCl_Bm_LOG.COM File for Running FMT in the DEC Environment

```
$ Set default [<root>. TEST_CASES.Np_NaCl_BM]
$ define INPUT Np_NaCl_BM_LOG.IN
$ define INGUESS Np_NaCl_BM_LOG.INGUESS
$ define CHEMDAT [<root>.HMW_DB]HMW_NP_AM_RTEST.CHEMDAT
$ define RHOMIN [<root>.HMW_DB]HMW_NP_AM_RTEST.RHOMIN
$ define OUTPUT Np_NaCl_BM_LOG.OUT
$ define FOR088 Np_NaCl_BM_LOG.FOR088
$ define TITRATE Np_NaCl_BM_LOG.TITRATE
$ run [<root>.FMT]FMT2P3.EXE
$ deassign INPUT
$ deassign OUTPUT
$ deassign CHEMDAT
$ deassign RHOMIN
$ deassign OUTPUT
$ deassign FOR088
$ deassign TITRATE
```

6.3.4 Macintosh Environment

The user double clicks with a mouse or track ball on the Macintosh executable icon for FMT, named PMacFmt. A screen titled "Output from PMacFmt" displays the file prompts and writes each file name on the screen after the user selects or names a file. The user makes a selection through a window display by navigating the folders or directory tree, double clicking on an input file name, and typing in the output file name or using the default file name.

The user can set a folder or directory before selecting or naming any file. The order of prompts directs the user to:

1. Select CHEMDAT File
2. Select RHOMIN File*
3. Select INPUT File
4. Select INGUESS File

---

* Although the RHOMIN file is not used for batch calculations, the user must still provide a file name for it when operating in a Macintosh environment.

5. Enter OUTPUT File Name

For a batch problem,

6. Enter FOR088 File Name

or

for a tritrate problem,

Enter TITRATE File Name,

7. Enter "Y" or "y" to echo data base in OUT file

6.4 Setting up and Running a Batch (Flash) Problem

The input files for batch problems are INPUT, INGUESS, and CHEMDAT. The user supplies the INPUT and INGUESS files. CHEMDAT is provided as a standard data base file.

In batch problems, FMT generates two output files: OUTPUT and FOR088.

6.4.1 Screen Display Descriptions

The lines displayed on the screen during the execution of batch problems are frequently repeated in the OUTPUT file, including the CHEMDAT portion of that file. Any error messages will be displayed on the screen and printed in the OUTPUT file. The user can refer to Section 8.0 for explanations of errors and other messages; the OUTPUT file is documented in Section 9.1.

Table 2 explains the lines displayed to the user's screen during FMT execution. The "Line" column refers to the line numbers listed in a display of the screen during execution of a sample problem called "BATCH_DOC." If applicable, the "Variable Name" column shows FMT program variables.

6.4.2 Using FOR088 File as INGUESS File

The secondary output file FOR088 is produced from batch runs. Using the FOR088 as an INGUESS file provides an easy way to adjust the solution composition.

Table 2. Batch Problem Screen Display Description (See Appendix A for sample listing.)

Line	Variable Name	Description
1	CHEMDAT_NAME	partial string of a CHEMDAT file name to search on
2	RHOMIN_NAME	partial string of a RHOMIN file name to search on
3	FILE_NAME	full file name without the ".xxx" extension
4-6		notation; setting pointers to FMT CMS library
8-13		list of CHEMDAT files with their comments in FMT CMS library that correspond to search string in line 1
14	CHEMDAT_NAME	user double clicks, cuts and pastes with a mouse, or types in appropriate CHEMDAT file name
15-18		notation indicating that the CHEMDAT file name in line 14 has been copied to the user's current directory
20-24		list of RHOMIN files with their comments in FMT CMS library that correspond to search string in line 2
25	RHOMIN_NAME	user double clicks, cuts and pastes with a mouse, or types in appropriate RHOMIN file name
26-29		notation indicating that the RHOMIN file name in line 25 has been copied to the user's current directory
30	DUMMY	user's response to echoing CHEMDAT parameters in the OUT file
32-36		linker and identity on building the FMT executable in CMS library
38	DUMMY2	FMT read 'nDG_BYPASS' from CHEMDAT file (HMW_NP_AM.CHEMDAT, Appendix I)
39		notation; repeat of line 1 of INPUT file (BATCH_DOC.IN, Appendix E) with 'FMT' and version number
40-45	DBASE1, DBASE2, ACCURACY, MINABU,NAQ	repeat of lines 4-9 OUTPUT file for CHEMDAT (Appendix J)
47	DUMMY2	FMT read 'PITZACT' from CHEMDAT file (Appendix I)

48-56		notation indicating Pitzer parameters being read from CHEMDAT file
57	ELNAMES (RPLWCHG)	repeat of line 1286 from OUTPUT file for CHEMDAT (Appendix J)
59	CDUM1,CDUM2	character strings read from line 4 of INPUT file (Appendix E) to set batch mode
60		notation that FMT has a BATCH problem
62	DUMMY, DUMMY1	character strings read from line 6 of INPUT file (Appendix E) to *not* read species amounts from INGUESS
63-86	ABUND(i), ELNAMES(i)	notation; listing of elemental abundances i^{th} mole amount starting at line 7 of INPUT file (Appendix E) and i^{th} element name starting at line 8 of CHEMDAT file (Appendix I)
87-96, 106-109	NAMES(i)	species deleted from equilibrium algorithm because their total number of moles NMOLES(i) became negligible (<MINABU×1×10^{-6})
98-105		repeat of lines 20-27 in OUTPUT file for Batch (BATCH_DOC.OUT, Appendix L)
110		repeat of line 166 in OUTPUT file for Batch (Appendix L)
111		repeat of line 171 in OUTPUT file for Batch (Appendix L)
112,113		repeat of lines 183, 184 in OUTPUT file for Batch (Appendix L)
114		notation; normal exit from batch mode

Each batch run generates the output files OUTPUT and FOR088. The FOR088 file contains the number of moles of each species calculated from the equilibrium run, normalized to a 1 kg H_2O basis. The user could rename the FOR088 file to INGUESS, change the flags to 'MOLES' 'EXACT' in INPUT, and recalculate the equilibrium solution using the species concentrations (total mole amounts) read from the renamed INGUESS file. In this scenario, the calculated results would be the same.

If a user wanted to use the calculated concentrations from BATCH_DOC as a starting point but, for example, wanted the solution to be less basic, one could take the new INGUESS file, and

increase the moles of one or several acids (or whatever else one desired to change) and run the problem again. Because the total mole amounts would be calculated from the INGUESS file, this would change the equilibrium concentrations. All changes to amounts in the INGUESS file must maintain charge-neutrality.

The process of running FMT, renaming the FOR088 file as the INGUESS file, modifying the INGUESS file, and rerunning FMT, can be used to fine tune the composition to whatever the user desires.

6.5 Setting up and Running a Titrate Problem

In addition to running in batch mode, FMT can calculate equilibrium concentrations resulting from titrating one solution with another solution or a solution containing minerals ("a slurry"). For titrate problems, the user defines two solution compositions, the solution to titrate with, called the titrant or the "buret" solution, and the solution to be titrated, or the "Erlenmeyer" solution. The user must also specify the volumes of buret solution to add to the Erlenmeyer solution, and the number of additions.

Titration can be conceptualized as a series of N_s beakers each containing 1 liter of the Erlenmeyer solution. A volume of titrant solution in milliliters ΔV_i, $i=1,\ldots,N_s$, is added to each beaker. The first volume addition is always zero, that is, $\Delta V_1 \equiv 0$. At each titration step the specified volume is added to each of the N_s beakers containing 1 liter of Erlenmeyer solution, and each beaker is reequilibrated.

6.5.1 Using Volume Options (LOG10, LINEAR, and ASREAD)

FMT provides the user three different methods for specifying the titrant volume. Table 3 shows each option, a description of each option, and the mathematical method used to calculate the volumes to be titrated with each of the N_s Erlenmeyer solutions.

Table 3. Titrate Options

Option	Description	Method
LINEAR	add the same constant titrant volume for each increment	ΔV_i=DV(2)× (i-1), i=2,…,N_s, where DV(2) is read from the INPUT file
LOG10	add titrant volumes that increase exponentially from the user specified minimum to maximum volumes, i.e., event changes in log space	ΔV_i=DV(2) × $e^{(i-2)R}$, i=2,…,N_s, with R= $\frac{\ln(DV(N_s)) - \ln(DV(2))}{N_s - 2}$, where DV(2) and DV($N_s$) are read from the INPUT file
ASREAD	add user specified titrant volumes	ΔV_i=DV(i), i=2,…,N_s, where DV(i) values are read from the INPUT file

A problem called "Np_NaCl_BM" is used to illustrate the input and output files as an example problem. All three methods are demonstrated below using the same buret and Erlenmeyer solution compositions and same number of beakers, N_s =15. For the example Np_NaCl_BM problem the initial volumes are

DV(1) = 0.0 mL for all three options

DV(2) = 0.1 mL for all three options.

The incremental volume is

ΔV_i = 0.1×(i-1) mL for 'LINEAR'

ΔV_i = 0.1 × exp[(i-2)R] with R=(ln(10.0)-ln(0.1))/13.0,

i=2,…,15 for 'LOG10'

and user-specified increments for 'ASREAD'.

The final volume is

DV(15) = 1.4 mL for 'LINEAR' option

DV(15) = 10.0 mL for 'LOG10' and 'ASREAD' options.

Figure 5 illustrates the LINEAR option. In the example shown in the figure, 15 different solutions are considered. The first beaker is a 1-liter Erlenmeyer solution with no titrant added, the second is a l-liter Erlenmeyer solution with 0.1 mL of titrant added, the third is a 1-liter Erlenmeyer solution with 0.2 mL of titrant added, and so on up to the last beaker, a 1-liter Erlenmeyer solution with 1.4 mL of titrant added.

The LOG10 option is particularly convenient for covering large concentration ranges, such as K_2CO_3 concentration from 0.001 to 5 molal.

The user can use the above options in the following order:

1. use the LOG10 option to rapidly find the full extent of pH response possible
2. use the LINEAR option to focus on regions of slow and rapid pH changes
3. use the ASREAD option to customize the placement of points.

All options use NSPACE, the number of Erlenmeyer solutions. The LINEAR option requires an initial volume DV(2). The LOG10 option requires initial and last volumes DV(2) and DVMAX. The ASREAD option requires DV(i) amounts defined by the user

where i=2, . . ., NSPACE.

When the flag for titrating (or "injecting") solids 'INJSOLIDS' is turned on, FMT will add both the aqueous phase and solid phase portions of the titrant solution as a slurry mixture. Otherwise, only the aqueous phase is added.

6.5.2 Screen Display Descriptions

Table 4 explains the lines displayed to the user's screen while executing FMT for the titrate problem. The "Line" column refers to the lines listed in screen displays of the Np_NaCl_BM_LOG, Np_NaCl_BM_LIN, and Np_NaCl_BM, the LOG10, LINEAR, and ASREAD runs of the titrate problem, which are described in detail later in this manual. "Variable Name" column shows FMT's program variables.

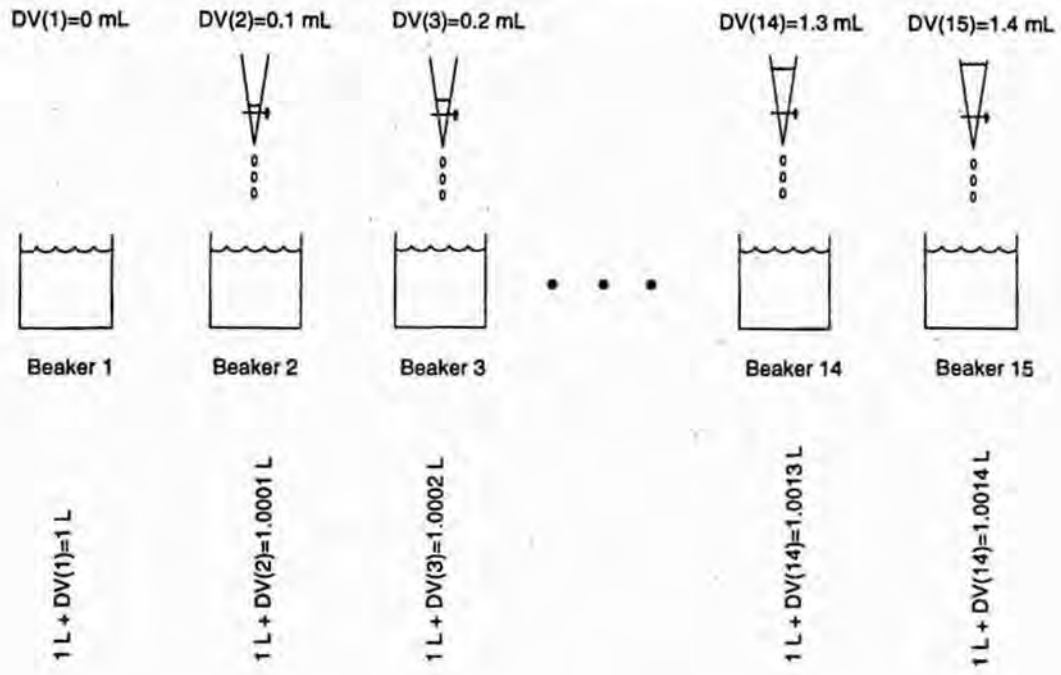


Figure 5. Titration problem using LINEAR option.

6.5.3 Titrate Sample Problem: Solubility Calculation

*****NOTE*****

The user should be familiar with the input and output files for the 'ASREAD' titration calculation (see Section 6.5.1) before reading this section.

The following example Np(V)/CO_3/NaCl problem illustrates a typical way in which FMT is used. This calculation is designed to show how the solubility of $NaNpO_2CO_3(s)$ varies as a function of CO_3^{2-} concentration in 5.61 molal NaCl media. This is the simulation used to generate Figure 7 of Novak and Roberts (1995). Because it is not possible to vary the carbonate concentration while keeping the concentrations of both Na^+ and Cl^- constant, the simulation was designed to keep the Na^+ concentration constant.

Referring to Appendix O, the listing for Np_NaCl_BM.OUT (an output file for the titrate calculation using the 'ASREAD' option), the flash calculation output for the titrant shows 5.61 molal sodium on Lines 324 and 368, approximately 2 molal CO_3^{2-} on Line 369, with 1.61 molal

Table 4. Titrate Problem Screen Display Description (See Appendices B, C, and D for sample screen displays of Np_NaCl_BM_LOG, Np_NaCl_BM_LIN, and Np_NaCl_BM, respectively.)

Line	Variable Name	Description
1-47, 49-59		repeat of variable names and descriptions in Table 2 for Batch for lines 1-47 and 48-58
48	DUMMY	notation that CHEMDAT parameters are not listed in the OUT file
60	CDUM1,CDUM2	character strings read from line 4 of INPUT (Np_NaCl_BM_LOG.IN [Appendix F], Np_NaCl_BM_LIN.IN [Appendix G], or Np_NaCl_BM.IN [Appendix H]) to set titrate mode
61		notation that FMT has a TITRATION problem
63	CDUM1,CDUM2	character strings read from line 6 of INPUT (Appendices F, G, or H) to *not* read species amounts from INGUESS for the injected or buret solution
64	CDUM1,CDUM2	character strings read from line 31 of INPUT (Appendices F, G, or H) to *not* read species amounts from INGUESS for the initial or Erlenmeyer solution
65		pH (negative base 10 logarithm of hydrogen ion activity) of the titrant solution and pmH (negative base 10 logarithm of hydrogen ion molality)
66		fugacity and logarithm of fugacity of CO_2 for titrant solution
67		pmH and pH of the Erlenmeyer solution
68		fugacity of CO_2 for Erlenmeyer solution
69, 70	CDUM1,CDUM2	character strings read from line 100 of INPUT (Appendices F, G, or H) to set titrate method
71, 72	DV(2), DV(NSPACE)	initial titrant volume as read from INPUT (Appendices F, G, or H) and final titrant volume; for example, 0.1 mL and 1.4 mL in Figure 5
74-103		first line is pH and pmH of resulting solutions following titrant additions DV(i), i=1, . . ., N_S to 1 liter of the Erlenmeyer solution, beginning with no additions to the first beaker; see Figure 5. Second line is fugacity of CO_2.
104		notation; normal exit from titrate mode

Cl^- (Lines 328 and 370) to create a charge-neutral solution. The titrant was designed to have a very high carbonate concentration. The solution could not have been made much more concentrated in carbonate because it is nearly saturated with respect to $Na_2CO_3 \cdot 7H_2O(s)$ as indicated by the Saturation Index of –0.251 listed in the Descriptor column on Line 379. The flash calculation output for the Erlenmeyer solution shows 5.61 molal sodium and 5.61 molal chloride (Lines 418 and 422), in equilibrium with a large excess of $NaNpO_2CO_3(s)$ at a relatively high pmH of 5.91 on Line 488. This solution was designed to have a very low carbonate concentration, 3.09×10^{-8} molal (Line 470). A large excess of $NaNpO_2CO_3(s)$ was specified because we are investigating the solubility behavior of this solid as conditions vary, and the large excess allows the amount of solid to change with changing aqueous conditions while keeping the solid phase present.

Examining the TITRATE file, Appendix S, the listing for Np_NaCl_BM.TITRATE on Lines 27-41, shows that the Na^+ concentration remains constant at 5.61 molal, while the Cl^- concentration changes slightly from 5.61 to 5.51 molal. More importantly, the CO_3^{2-} concentration varies widely, from 3.09×10^{-8} to 4.84×10^{-2} molal (Lines 44-58), as was intended. The $NaNpO_2CO_3(s)$ concentrations confirm that this solid is present across this aqueous composition range (Lines 112-126), and all other solid phases are absent. The concentrations of the Np(V) species NpO_2^+, $NpO_2OH(aq)$, $NpO_2(OH)_2^-$, $NpO_2CO_3^-$, $NpO_2(CO_3)_2^{3-}$, and $NpO_2(CO_3)_3^{5-}$, given in Lines 95-109 are the desired information from this simulation; these are plotted in Figure 6, along with the total Np(V) in solution (the sum of the individual species concentrations) and experimental measurements of this system from Neck et al. (1994).

The data from Neck et al. (1994) plotted in Figure 6 are:

mCO_3^{2-}	mNp(V) total		mCO_3^{2-}	mNp(V) total
9.49E-4	5.13E-6		3.61E-3	1.07E-5
3.61E-4	4.17E-6		6.27E-3	2.24E-5
7.20E-5	4.47E-6		1.50E-2	8.51E-5
9.93E-6	1.15E-5		1.98E-2	1.38E-4
2.38E-6	3.39E-5		2.74E-2	2.57E-4
1.25E-6	6.17E-5		1.09E-3	4.47E-6
3.78E-7	2.04E-4		3.29E-4	3.55E-6
1.73E-7	4.37E-4		2.50E-4	3.63E-6
1.57E-7	4.90E-4		2.28E-5	6.46E-6
9.06E-6	1.29E-5		6.27E-7	1.41E-4
2.74E-5	6.17E-6		5.72E-8	1.10E-3
1.19E-3	4.90E-6			

Figure 6 is comparable to Figure 7 from Novak and Roberts (1995), the main difference being the axis ranges. This figure shows that the hydrolysis species $NpO_2OH(aq)$ and $NpO_2(OH)_2^-$ are unimportant under these conditions, with concentrations always at least three orders of magnitude smaller than the total Np(V). This example shows the comparison between model calculations and experimental data, and also shows that the values calculated with FMT Version 1.0, used in Novak and Roberts (1995), agree with values calculated with FMT Version 2.3, used in this user's guide. The symbols in the calculated curves serve both to identify the individual curves and show the positions of the flash calculations used to define the curves. If desired, one could trace these calculated species concentrations to values in Appendix S.

Figure 6 also shows how the 'ASREAD' option for titration problems lets the user specify exactly where values for the independent variable, in this case CO_3^{2-} concentration, will be. The modeling points were spaced relatively far apart in regions with linear behavior and closer together in regions of curvature.

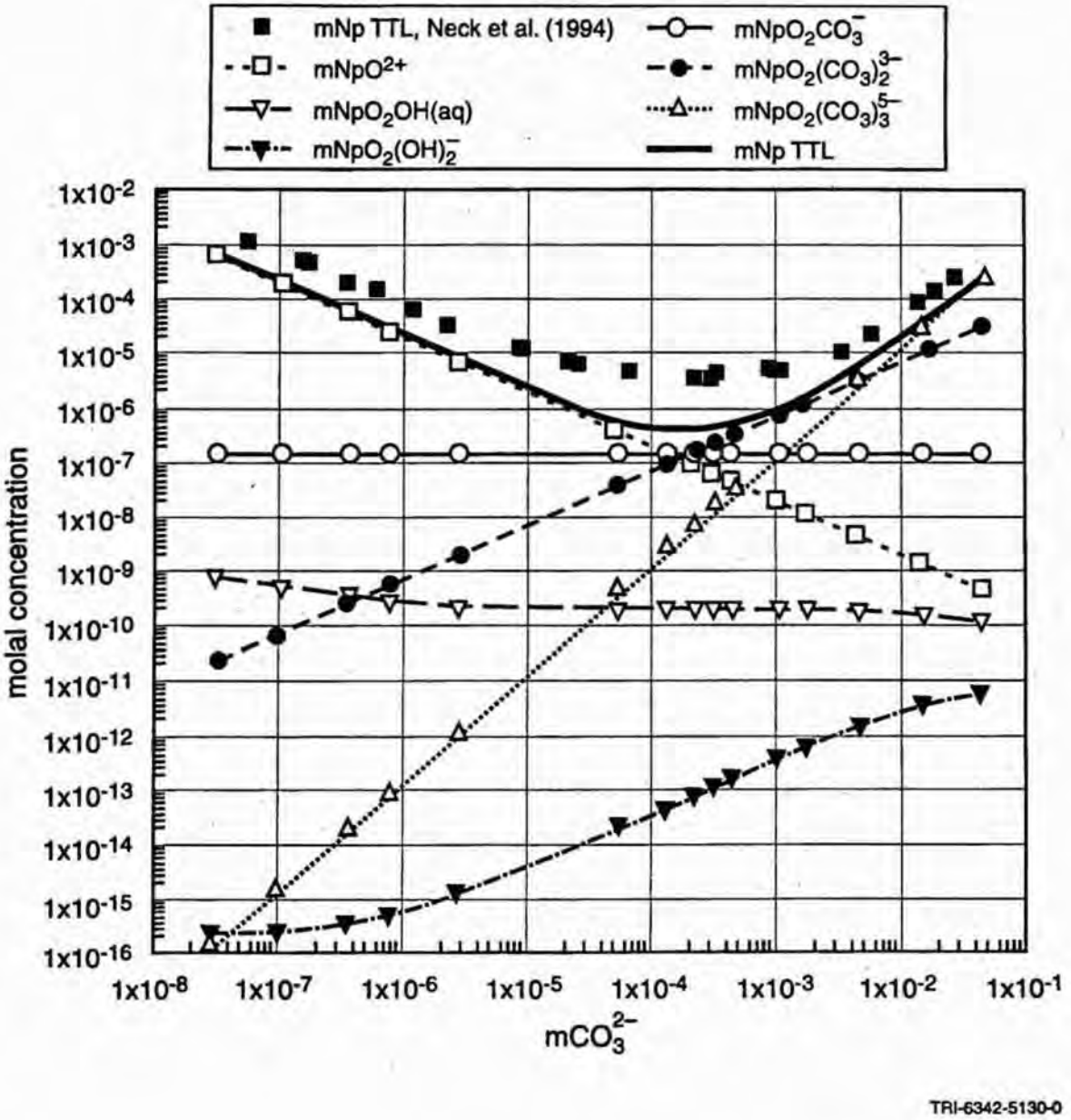


Figure 6. Calculated Total Np(V) and Np(V) Concentrations as a function of CO_3^{2-} concentration in 5.61 molal (5M) NaCl, and comparison with experimental measurements from Neck et al. (1994).

7.0 DESCRIPTION OF INPUT FILES

Of the three or four input files for FMT (see Figures 1 and 2), the user provides two files (INPUT and INGUESS). The other files (CHEMDAT) or (CHEMDAT and RHOMIN) are the input data base files and are supplied by the code authors. INPUT and INGUESS can be edited with any convenient text editor.

The input data files are read using standard FORTRAN free-field format read conventions. All character data must be enclosed in single quotes. Data are separated by either a space or a comma. Blank lines may be inserted anywhere in the input files to improve readability.

Comments are interspersed throughout the input files. These are not read by FMT and they are placed at the end of a line. They are used to:

- identify the element or species on a line, or
- document the reference source of data on a line.

FMT uses character strings to set options or flags in the INPUT and CHEMDAT files. The following options are considered:

- "on" when the character string equals a specific set of upper case letters, such as 'MOLES' or 'BATCH', or
- "off" when the character string equals any other set of letters.

The code developer of FMT chose to indicate turning "off" options by placing a lower case "n" before the specific string that turns an option "on," e.g., 'nMOLES' or 'nBATCH'. This offers the advantage of keeping the meaningful value of the flag close at hand for easy interpretation of the individual flags.

Batch problems require the input files INPUT, INGUESS, and CHEMDAT to run, and an additional file RHOMIN is required for titrate problems. A description of all four input files, for both Batch and Titrate calculations, follows.

7.1 INPUT

7.1.1 Batch Problem

The batch INPUT (.IN) file is used to specify the molar abundances of the elements for the batch problem. The bulk of the lines in this file (Figure 7) specifies element abundances. The flags on Line 6 indicate if the INGUESS file should be read for species abundances. A line-by-line description of this file is provided below in Table 5, and a sample listing of BATCH_DOC.IN is provided in Appendix E.

Table 5 lists the INPUT file parameters for a batch problem. The "LINE" column refers to the line numbers listed in the BATCH_DOC.IN file. The "Variable Name" column corresponds to the FMT program variables. "Permissible Value" column is the only set of values permitted for use with this program. Any other values have unknown consequences.

As shown in BATCH_DOC.IN file on lines 7-29, each amount is followed by an element or a psuedoelement name. The names are not read by FMT and are included for human readability only.

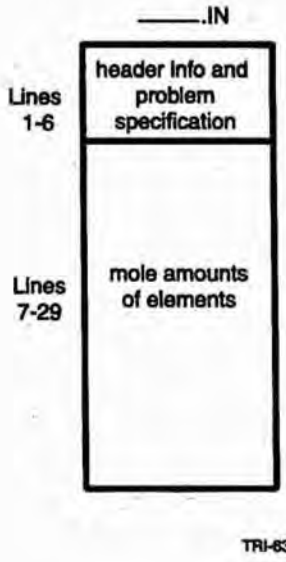


Figure 7. Batch INPUT file.

Table 5. INPUT File Parameters for Batch (See Appendix E for sample listing.)

Line	Variable Name	Permissible Value	Description
1	TITLE78	any character string (maximum 78 characters)	character string that identifies or describes the user's problem
2	DUMMY	'CHEMFILE'	character string used as a flag for reading the CHEMDAT file (Appendix I)
4	CDUM1, CDUM2	'BATCH' 'UNUSED'	the first string indicates this is a batch problem with the second string's value being irrelevant
6	DUMMY, DUMMY1	'MOLES' 'EXACT'	two character strings used as flags for calculating the equilibrium state using either: species abundances read from INGUESS from which FMT calculates element abundances
		or	
		'nMOLES' 'nEXACT'	element abundances from INPUT (does not read INGUESS)
7-29	ABUND (i)	nonnegative real number	mole amount of i^{th} element in the order listed in CHEMDAT (Appendix I, lines 8-10), one elemental amount per line

7.1.2 Titrate Problem

The titrate INPUT (.IN) file is used to specify the molar abundances of the elements for both the buret and Erlenmeyer solutions, along with the number of titrant volumes ("burets") that are to be added for the titrate problem. (See Section 6.5 for explanation of titration problem.) The bulk of the lines in this file (Figure 8) specify the molar abundances of the elements in the buret and Erlenmeyer ("beaker") solutions. Lines 6 and 31 allow the user to set flags to read the INGUESS file for species abundances. Line 100 allows the user to specify the titration method:

- LINEAR, adding equal volumes of the titrant successively,
- LOG10, adding titrant volumes that increase exponentially,
- ASREAD, adding user-specified titrant volumes.

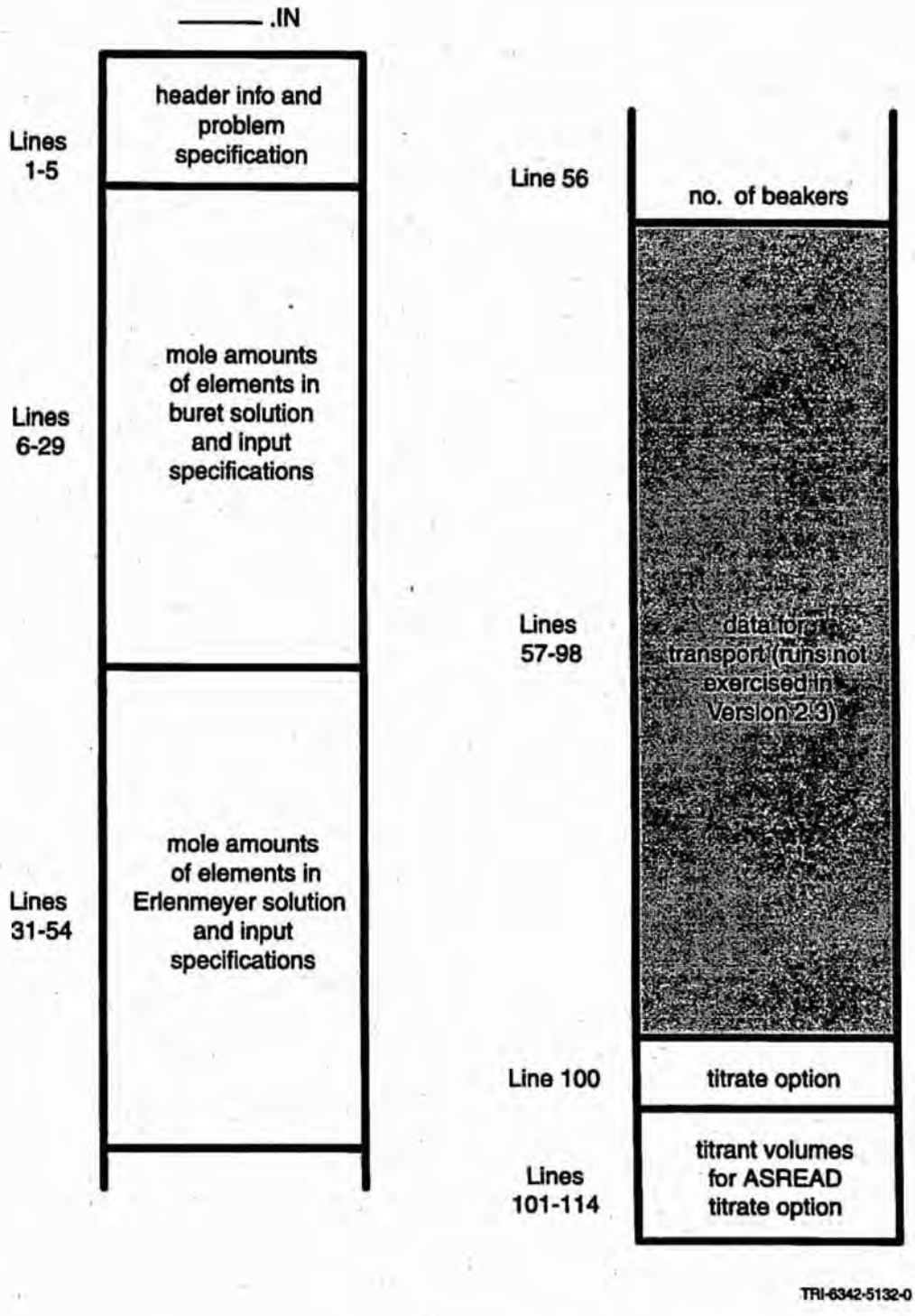


Figure 8. Titrate INPUT file.

The INPUT file parameters for a titrate problem are shown in Table 6. The "LINE" column in Table 6 refers to the lines listed in the Np_NaCl_BM_LOG.IN, Np_NaCl_BM_LIN.IN, and Np_NaCl_BM.IN files. Sample listings of these files are provided in Appendices F, G, and H.

In the input files referenced in Table 6, lines 7-29 state the composition of the titrant or buret solution. Lines 32-54 define the composition of the titrated or Erlenmeyer solution. Lines 6 and 31 are flags for reading the INGUESS file. Line 56 states the number of beakers, N_s, for titration. Lines 57 through 98 are read but not used.

Line 100 in the INPUT file demonstrates setting each of the three titration methods:

- Np_NaCl_BM_LOG.IN file (Appendix F) sets the 'LOG10' option with the initial and final volumes. FMT disregards any lines following line 100.

- Np_NaCl_BM_LIN.IN file (Appendix G) sets the 'LINEAR' option and the initial volume, and FMT disregards the final volume number. FMT stops reading the file and disregards any further lines.

- Np_NaCl_BM.IN file (Appendix H) sets the 'ASREAD' option, and FMT disregards the initial and final volume numbers. In lines 100-114 of this file, FMT reads the 14 user-specified volumes for the 'ASREAD' option.

7.2 INGUESS

The INGUESS file is a required input file for both the batch and titrate runs that allows the user to specify the species abundances, from which FMT calculates the element abundances. The user must set the flags to 'MOLES' and 'EXACT" in the INPUT file for FMT to read the INGUESS file. If the file is not read, a null can be used as the INGUESS file. The element abundances are read from the INPUT file.

7.2.1 Batch Problem

The user can rename the FOR088 output file from a batch calculation and modify the species amounts as desired to build a solution composition for the INGUESS file (see Section 6.4.2). A line-by-line description of the INGUESS file, whose structure is identical to that of the FOR088 file (Appendix P), is provided below in Table 7.

Table 6. INPUT File Parameters for Titrate (See Appendices F, G, and H for sample listings of Np_NaCl_BM_LOG.IN, Np_NaCl_BM_LIN.IN, and Np_NaCl_BM.IN, respectively.)

Line	Variable Names	Permissible Values	Description
1	TITLE78	any character string (maximum 78 characters)	character string that identifies or describes the user's problem
2	DUMMY	'CHEMFILE'	character string used as a flag for reading the CHEMDAT file (Appendix I)
4	CDUM1,CDUM2	'TITRATE' 'EXPLICIT'	the first and second strings are required to indicate that this is a titrate problem
6	CDUM1,CDUM2		two character strings used as flags for the titrant or buret solution for calculating the equilibrium state using either:
		'MOLES' 'EXACT'	species abundances read from INGUESS from which FMT calculates element abundances
		or	
		'nMOLES' 'nEXACT'	element abundances from INPUT (does not read INGUESS)
7-29	ELTOTAL (i,1)	nonnegative real number*	mole amount of i^{th} element in buret solution, one elemental amount per line
31	CDUM1,CDUM2		two character strings used as flags for the solution to be titrated or Erlenmeyer solution for calculating the equilibrium state using either:
		'MOLES' 'EXACT'	species abundances read from INGUESS from which FMT calculates element abundances
		or	
		'nMOLES' 'nEXACT'	element abundances from INPUT (does not read INGUESS)
32-54	ELTOTAL (i,2)	nonnegative real number**	mole amount of i^{th} element in Erlenmeyer solution, one elemental amount per line

* The value on line 29, though negative, is essentially zero since it is so small (order of magnitude: 10^{-15})

** The value on line 54, though negative, is essentially zero since it is so small (order of magnitude: 10^{-15})

56	NSPACE, TEMP,TEMP, TEMP, CDUM1	2 < integer number < 66 2.25d3 0.0025d0 1.800001d5 'nDXVARIABLE'	the first number in this line specifies the total number of beakers, N_s. Recall that the first beaker gets zero addition of titrant solution, so N_s-1 volumes are added. The three remaining numbers and character string should be specified as indicated, but these values are not used for titration problems.
57-98		exactly as specified in the INPUT (.IN) file	none of these values is used for titrate problems, but must be included
100			The following five values on this line set one of the titrate options:
	CDUM1	'TITRATE'	'TITRATE' must always read 'TITRATE'
	CDUM2		Specifies the method of adding volume amounts to each beaker:
		'LINEAR' or	add equal sequential volumes
		'LOG10' or	add exponentially increasing volumes
		'ASREAD'	read volume amounts from the INPUT file
	DV(2)		initial volume, in mL, to add to the second beaker, valid for LINEAR or LOG10 options. A value must exist but not used for ASREAD option.
	DVMAX		volume added to the last beaker, valid only for LOG10 option. A value must exist but not used for ASREAD or LINEAR options.
	CDUM3	'nINJSOLIDS' or 'INJSOLIDS'	By default, FMT will add only the aqueous phase part of the titrant to the Erlenmeyer solution. However, if the user wishes to add both the aqueous phase and solid phase portions of the titrant solution, which can be conceptualized as a slurry, this option for titrating (or "injecting") solids is turned on with the flag 'INJSOLIDS'

101-114	DV(i)	nonnegative real number	read titrant volumes, in mL, to be added for each of the N_s-1 additions where N_s value is set on line 56. For the ASREAD option; see Appendix H for illustration. For the LINEAR and LOG10 options, the INPUT file is not read after line 100.

Table 7. INGUESS File Parameters for Batch Problem

Line	Variable Name	Permissible Value	Description
1-115	NMOLES (i)	nonnegative real number	mole amount of i^{th} species in the order listed in CHEMDAT (Appendix I, lines 14-140), one species amount per line

On each line of an INGUESS (from an FOR088) file, the total moles normalized to a 1 kg H_2O basis are followed by a species name and the number of moles of that species, based on the abundances from which the file was generated. FMT reads only the first column or first number on each line from an INGUESS file. The order of the species listed follows that of the CHEMDAT file (Appendix I, Lines 14-140). HMW_NP_AM_RTEST.CHEMDAT file has 115 species.

7.2.2 Titrate Problem

When running a titrate problem, a user could direct FMT to compute the total element abundances for either the buret or Erlenmeyer solution by setting one set of species abundances in the INGUESS file and 'MOLES' 'EXACT' in either line 6 or 31 in the INPUT file as listed in Table 6. 'MOLES' and 'EXACT' set on line 6 would use INGUESS for buret solution; MOLES' and 'EXACT' set on line 31 would use INGUESS for the Erlenmeyer solution. Table 8 describes the INGUESS file parameters for a titrate problem.

Table 8. INGUESS File Parameters for Titrate Problem

Line	Variable Name	Permissible Value	Description
1-115	NMOLES (i)	nonnegative real number	mole amount of i^{th} species listed in CHEMDAT (Appendix I, lines 14-140), one species amount per line, for buret or Erlenmeyer solution

7.3 Standard CHEMDAT Input File

FMT calculates the equilibrium state of an aqueous/mineral system using the HMW data base system, as specified in the CHEMDAT file. HMW stands for Harvie-Møller-Weare/Felmy-Weare (Harvie et al., 1984; Felmy and Weare, 1986); it represents a thermodynamic model for evaporite systems using the Pitzer activity coefficient formalism (Section 4.2). The WIPP Project has extended this brine data base to include some actinides.

The term HMW_NP_AM_RTEST.CHEMDAT as used throughout this document refers to version 95.01.31 (created January 31, 1995) of the file (a copy and output list of which are provided in Appendices I and J, respectively) where:

- HMW stands for Harvie-Møller-Weare/Felmy-Weare
- NP stands for neptunium(V)
- AM stands for americium(III)
- RTEST stands for a format modification for use in regression testing of FMT 2.3.

The elemental list in the CHEMDAT file contains the physical elements as found on the periodic table and "psuedo elements" as required for solving chemical equilibrium problems. The psuedo elements in the HMW_NP_AM_RTEST.CHEMDAT file are PosIon, NegIon, Air, Boron, Bromine, TracerEl, ClO4-(EL), Electron and Charge. These psuedo elements are treated exactly like the physical elements in the mathematical sense, regardless of their identity. See Section 4.5.

The CHEMDAT file illustrated throughout this document is HMW_NP_AM_RTEST.CHEMDAT, version date 95.01.31.

NOTE
HMW_NP_AM_RTEST.CHEMDAT is not the CHEMDAT file that was used to support the WIPP PA calculations. Additional species and elements were added to support the WIPP PA calculations.

This data base contains an early set of thermodynamic parameters for modeling the chemical behavior of Np(V) and Am(III) in brines. Note that the extension of the Pitzer model to higher electrolyte types than in Harvie et al. (1984) and Felmy and Weare (1986) is necessary for Am(III); this is discussed in Pitzer and Silvester (1978).

WARNING
The user should not and is not expected to change the CHEMDAT file. To do so invalidates the QA performed on this data base.

7.3.1 CHEMDAT Data Flow

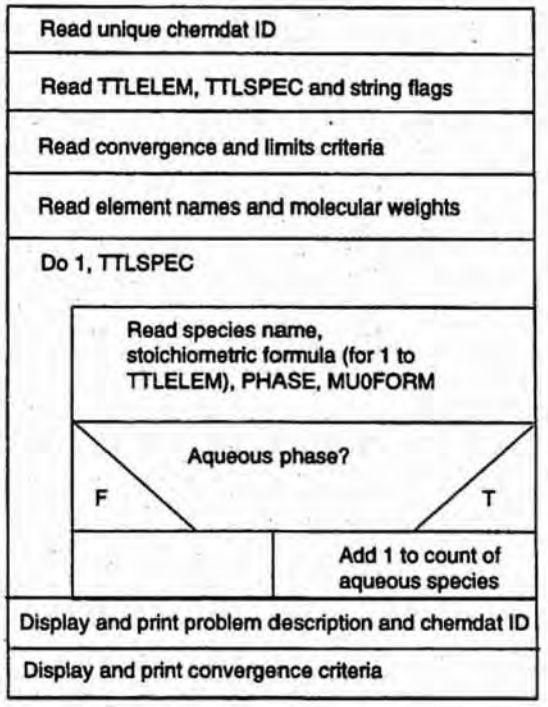
Both FMT subroutines READDAT and RDPITZR read from the CHEMDAT file. If the user responds with a y or Y (yes) to the question, "Echo data base in the OUTfile" (see sections 6.3.2.2 and 6.3.4), parameters read from CHEMDAT are echoed or printed to the OUTPUT file. Some parameters are also displayed on the user's screen.

The FMT control flow is illustrated with a Nassi-Schneiderman (N-S) chart (Figure 9). This shows the data flow of the CHEMDAT file in the READDAT subroutine. FMT program variables TTLELEM and TTLSPEC in the diagram are the total number of elements and the total number of species, respectively.

7.3.2 Data Sources for HMW_NP_AM_RTEST.CHEMDAT

The thermodynamic data in HMW_NP_AM_RTEST.CHEMDAT can be grouped into three types: parameters for the brine electrolytes, parameters for Np(V) species and Np(V) species interactions with the brine electrolytes, and parameters for Am(III) and Am(III) species interactions with the brine electrolytes. All data are formally applied at 25°C although some data were taken at 25±5°C.

The data for the brine electrolytes were taken from Harvie et al. (1984) and Felmy and Weare (1986), as specified earlier, with some additional information on the perchlorate ion taken from Pitzer (1991). The data for Np(V) were taken from the old data base of Novak and Roberts



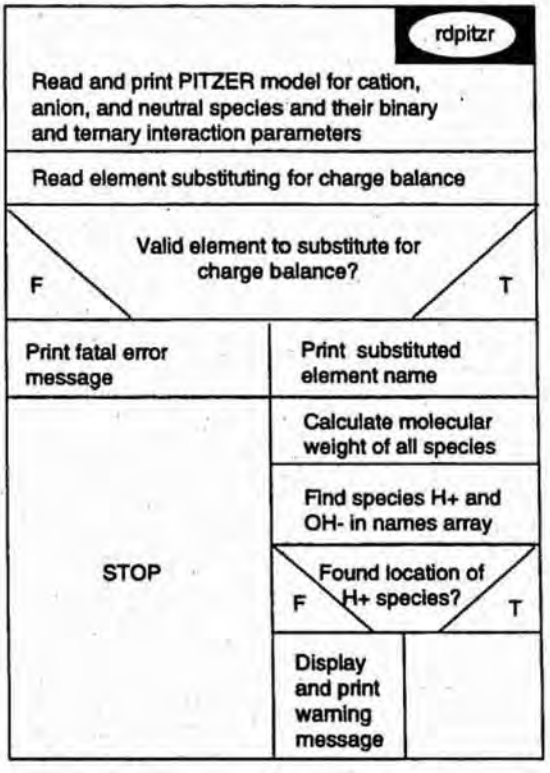


Figure 9. Nassi-Schneiderman (N-S) chart showing FMT control flow.

(1995), which has been superseded by newer work. We retain this older set of data to satisfy quality assurance and regression testing procedures only. We do not recommend the use of the Np(V) parameters from Novak and Roberts (1995). The Am(III) data contained in HMW_NP_AM_RTEST.CHEMDAT is taken from Felmy et al. (1990), Felmy et al. (1989), Rai et al. (1992a, 1992b, 1994), and Rao et al. (1994). These also represent an older set of thermodynamic data and as such is not as complete as the set of data in the most recent data base release, HMW_Am3Pu3Th4Np5_960823.CHEMDAT, as discussed in Appendix V.

7.3.3 Description of the HMW_NP_AM_RTEST.CHEMDAT File

The standard chemical potentials for most species are values obtained from a reference source, as explained in Section 7.3.2. At the end of some lines shown in the listing of HMW_NP_AM_RTEST.CHEMDAT in Appendix I, the character strings FRSR89, FRF90, PS76, P91, RFF92, RFFR92, RFF94, RRFF94, NR94, HMW84, and FW86 indicate the source of the data. The key to citations is listed at the end of the file in Appendix I. These indicators are not read by FMT, but serve merely to help with human interpretation of the file.

The standard chemical potentials for some species, i.e., lines 39-49 and 70-72 in Appendix I, are described as "arbitrary." The Table 9 lists the value, the lines where instances occurred, and the definition of the value.

Table 9. Arbitrary Values Used for Standard Chemical Potentials

Arbitrary Values	Example in Lines	Definition
-999.99	39, 40, 70, 72	physical species that represent the only occurrence for that element, i.e., no chemical reactions possible with the data base as specified
0	45, 46, 49	nonphysical species; included to facilitate the running of certain types of problems
500.	42, 43, 44, 47, 48	species included for adjusting the hydrogen ion concentration when setting up an input file, designed to completely dissociate within an equilibrium problem
999.99	77	species that may be added in future, but which are not allowed to form in a solution (the character string DISABLED is appended to their name)

The nonphysical species are included for convenience only. For example, they facilitate the addition of HCl(aq) to adjust the pH. To make sure these species are never calculated as being present, they have been arbitrarily assigned the large positive value 500 for dimensionless standard chemical potential.

In Table 10 the "Variable Name" column is for the FMT program variables. Input parameters that are described as unused are not supported in this version of FMT.

Table 10. CHEMDAT Input Parameters (Listing of HMW_NP_AM_RTEST.CHEMDAT provided in Appendix I.)

Line	Variable Name	Description
1-2	DBASE1, DBASE2	unique identification of the data base
4	TTLELEM, TTLSPEC, DUMMY, DUMMY2, DUMMY1, DUMMY3	number of elements (positive integer); number of species (positive integer); unused flag; unused flag; extra echo printing flag (if user specifies 'ECHO,' then extra information will be printed); unused flag
5	MAXIT, ACCURCY, MINABU	maximum number of iterations for each equilibrium calculation (positive integer); convergence tolerance on equilibrium problem (positive, real); minimum element abundance, abundances below which elements are considered not to be there (positive, real)
6	DUMMY, TEMPERA, P(1), P(2)	character flag indicating the units for standard chemical potentials ('NONE' means dimensionless); temperature in degrees Kelvin (real, positive); unused pressure in atmospheres, unused pressure in atmospheres. Note: TEMPERA is always set to 298.15 by FMT.
8-10	ELNAMES(i)	name of i^{th} element
11-12	MWELEM(i)	molecular weight of i^{th} element

14-140	NAMES(j), FORMULA(i,j), PHASE(j), MU0FORM(j)	name of j^{th} chemical species; stoichiometric number of each element in the species and charge of species (last number); phase of the species (1=aqueous, 2=solid); standard chemical potential of the species (in the units indicated by the flag in line 6). Entries in the formula vector usually are, but need not be, integers, and can be positive or negative. H_2O must always be the first species declared. All aqueous species must be declared before any solid species is declared.
142	DUMMY2, ITEMP	character flag that, when set to 'DG_BYPASS' allows alternate values for the standard chemical potentials to be read from file "bypass" for the first ITEMP species.
143	DUMMY2	character flag that enables the use of the Pitzer activity coefficient model when equal to 'PITZACT'. Any other character string will disable the Pitzer activity coefficient model.
144	NCATION	number of cations for which Pitzer activity coefficient model is used (positive integer) See note below Line 862 for a discussion of the order of cations, anions, and neutral species.
145	NANION	number of anions for which Pitzer activity coefficient model is used (positive integer)
146	NNEUTRL	number of neutral species for which Pitzer activity coefficient model is used (positive integer)
148-419	SE(i,j,1)	array of single electrolyte parameters The notation for charges on each cation-anion interaction is 1 when either cation or anion has a charge of 1 2 when both cation and anion have a charge of 2 3 for all other cases.
	SE(i,j,2)	$\beta^{(0)}$ parameter for each cation-anion interaction
	SE(i,j,3)	$\beta^{(1)}$ parameter for each cation-anion interaction
	SE(i,j,4)	$\beta^{(2)}$ parameter for each cation-anion interaction

	SE(i,j,5)	C^{ϕ} parameter, but this is later converted to C_{MX} (see equation A.4b, Harvie et al. [1984] or equation 2b, Felmy and Weare [1986], which is reproduced in Section 4.3).
		Note on cation-anion interactions: the parameters for SE are read in order - the first cation for all anions, then the second cation for all anions, etc. The character strings at the end of the numbers indicate the cation-anion pair specified on each line, for ease of human interpretation only.
422-433	ME(i,j,1)	for i>j, i and j are cation indices, cation-cation ternary interactions, θ_{ij}
436-454	ME(i,j,1)	for i<j, i and j are anion indices, anion-anion ternary interactions, θ_{ij}
456-544	PSI(i,j,k)	for i>j, i and j are cation indices, k is the anion index, cation-cation-anion ternary interactions, Ψ_{ijk}
546-753	PSI(i,j,k)	for i<j, i and j are anion indices, k is the cation index, anion-anion-cation ternary interactions, Ψ_{ijk}
755-760	NEUCAT(i,j)	neutral-cation binary ion interaction parameters, i=neutral species index, j=cation index, λ_{ij}
762-767	NEUANI(i,j)	neutral-anion binary ion interaction parameters i=neutral species index, j=anion index, λ_{ij}
769-851	PTZTSI(i,j,k)	neutral-cation-anion ternary ion interaction parameters, i=neutral species index, j=cation index, k=anion index, ζ_{ijk}
853-855	ELMAP(1,i)	maps the location in the species list to the order the Pitzer parameters were entered (read in groups of 6): cation map
857-860	ELMAP(2,i)	anion map
862	ELMAP(3,i)	neutral species map

		Note on species order: cationic, anionic, and neutral species are referenced by the order given in ELMAP(,). This is determined as follows: the cations are the second, third, fourth, fifth, sixth, seventh, twenty-second, etc., species entered in the species list, i.e., Na^+, K^+, Ca^+, Mg^+, $MgOH^+$, H^+, $MgB(OH)_4^+$, etc. Similar patterns are used for anions and neutral species. This allows additional flexibility in reorganizing and rearranging the data input files without having to reenter all of the ion interaction parameters. Although the order is arbitrary, it is very important that a consistent order is maintained throughout the CHEMDAT file. Because all parameters are clearly labeled, the echo printing of the ion interaction parameters makes is easy to determine whether errors were made when changing the CHEMDAT file. *****CAUTION***** **THE USER MUST NOT ALTER THE CHEMDAT FILE WHEN IT IS BEING USED FOR WIPP PA CALCULATIONS.**
864	DUMMY, NEQACT	character flag that, when equal to 'EQUALACT', indicates that NEQACT (positive integer) activity coefficients of "nonPitzer" species will be set equal to activity coefficients of Pitzer species. For example, one could run calculations using both ^{22}Na and ^{23}Na (which would have to be declared as separate elements in the element list), but instead of repeating all the ^{23}Na parameters for ^{22}Na, use the 'EQUALACT' flag. When DUMMY='EQUALACT' this line would be followed by NEQACT pairs of positive integers, one pair per line, corresponding to species position in the species list. The activity coefficient of the first species in the pair will be set equal to the activity coefficient of the second species of the pair.
866	RPLWCHG	positive integer indicating the element to RePLace With CHarGe. Used to implement the constraint of solution charge neutrality. The 2nd element corresponds to oxygen.
867	DUMMY, NEHRXN	character flag indicating whether redox reactions are specified (they are when the flag is 'REDOX'). When this flag is used, it will be followed by specifications of NEHRXN (positive integer) redox reactions. This feature is unsupported in FMT 2.3.

868	DUMMY, NSBSTPM, NSBSTRX, DUMMY1	flags and parameters for specifying ion exchange reactions. The value 'IONEX' means that ion exchange reactions are specified on NSBSTPM permanent substrates and NSBSTRX reactive (soluble) substrates. The value for DUMMY1 indicates what type of mass-action model to use for ion exchange calculations. This feature is unsupported in FMT 2.3.

7.3.4 Description of OUTPUT Listing of HMW_NP_AM_RTEST.CHEMDAT

The lines echoing the CHEMDAT file listed in Appendix J were taken from the output file, "BATCH_DOC.OUT". Table 11 explains the CHEMDAT portion. The OUTPUT file for a titrate problem will have the notation, "This is a TITRATION problem" for line 1289 and one less line, because line 1291 will be omitted.

Table 11. OUTPUT File Description of CHEMDAT Input Parameters (See listing provided in Appendix J.)

Line	Variable Name	Description
1		CHEMDAT file name
2		notation; FMT sets temperature to 298.15 Kelvin
3	TITLE99	problem title specified on line 1 of INPUT file with 'FMT' and version number appended
4-5	DBASE1, DBASE2	unique identification specified on lines 1 and 2 of CHEMDAT file
7	ACCURCY	convergence tolerance for equilibrium calculations, specified on line 5 of CHEMDAT file
8	MINABU	minimum elemental abundances for equilibrium calculations, specified on line 5 of CHEMDAT file. If the total number of moles of an element falls below this value, the element is considered to be absent (see Novak, 1995a).
9	NAQ	number of aqueous species in CHEMDAT
12		notation; species listed in order for Pitzer parameters
14-18	NCATION, NAMES (ELMAP(1,i))	cation species: count followed by an ordered list

20-25	NANION, NAMES (ELMAP(2,i))	anion species: count followed by an ordered list
27-29	NNEUTRL, NAMES (ELMAP(3,i))	neutral species: count followed by an ordered list
33-308		table of cation-anion binary interactions and parameters
	NAMES (ELMAP(1,i))	"Cation" species column
	NAMES (ELMAP(2,j))	"Anion" species column
	SE(i,j,2)	"Beta(0)" column, $\beta^{(0)}$ parameter for i^{th} cation, j^{th} anion interaction
	SE(i,j,3)	"Beta(1)" column, $\beta^{(1)}$ parameter for i^{th} cation, j^{th} anion interaction
	SE(i,j,4)	"Beta(2)" column, $\beta^{(2)}$ parameter for i^{th} cation, j^{th} anion interaction
	SE(i,j,5)	"Cphi" column, C^{ϕ} parameter for i^{th} cation, j^{th} anion interaction
	ALPHACH (SE(i,j,1))	"Alpha-Values" column (α_1 , α_2) string that states electrical charges on the i^{th} cation, j^{th} anion interaction (see Table 10, lines 148-419)
310-350		table of cation-cation ternary interactions and parameters
	NAMES (ELMAP(1,j))	up to ten columns of cation names on a line after leading cation
	NAMES (ELMAP(1,i))	name of leading i^{th} cation in the order listed on lines 16-18
	ME(i,j,1)	cation-cation ternary interaction parameter, θ_{ij}
353-428		table of anion-anion ternary interaction and parameters
	NAMES (ELMAP(2,j))	up to ten columns of anion names on a line after leading anion
	NAMES (ELMAP(2,i))	name of leading i^{th} anion, in the order listed on lines 22-25
	ME(i,j,1)	anion-anion ternary interaction parameters, θ_{ij}

431-591		table of cation-cation-anion ternary interaction and parameters
	NAMES (ELMAP(2,k))	up to ten columns of anion names on a line
	NAMES (ELMAP(1,i)), NAMES (ELMAP(1,j))	two cation names
	PSI(i,j,k)	cation-cation-anion ternary interaction parameter, Ψ_{ijk}
593-977		table of anion-anion-cation ternary interaction and parameters
	NAMES (ELMAP(1,k))	up to ten columns of cation names on a line
	NAMES (ELMAP(2,i)), NAMES (ELMAP(2,j))	two anion names
	PSI(j,i,k)	anion-anion-cation ternary interaction parameter, Ψ_{ijk}
979-994		table of neutral-cation binary interaction and parameters
	NAMES (ELMAP(3,i))	up to ten columns of neutral species names on a line
	NAMES (ELMAP(1,j)), NEUCAT(i,j)	j^{th} cation name and up to ten binary interaction values, λ_{ij}
997-1019		table of neutral-anion binary interaction and parameters
	NAMES (ELMAP(3,i))	up to ten columns of neutral species names on a line
	NAMES (ELMAP(2,j)), NEUANI(i,j)	j^{th} anion name and up to ten binary interaction values, λ_{ij}
1021-1284		table of neutral-cation-anion ternary interaction and parameters

	NAMES (ELMAP(3,i))	up to ten neutral species names in columns on a line
	NAMES (ELMAP(1,j)), NAMES (ELMAP(2,k))	j^{th} cation and k^{th} anion names
	PTZTSI(i,j,k)	up to ten ternary interaction values, ζ_{ijk}
1285		notation that Pitzer activity coefficient model is used
1286	ELNAME (RPLWCHG)	states name of element replaced by charge balance (see Table 10, line 866)
1289		notation that the problem is BATCH (If this were a titration problem, notation would be that the problem is TITRATION.)
1291		FOR088 file name for batch problem; line omitted if titrate problem
1293		notation that FMT uses dimensionless gas constant
1294	TKELVIN	temperature in degrees Kelvin, same as TEMPERA
1297	ALLSPEC, TTLELEM	number of species, number of elements
1299-1322	ELNAMES(i), MWELEM(i)	name and molecular weight of i^{th} element
1325-1440		listing of each species' chemical properties
	i, NAMES(i)	number and name of i^{th} chemical species
	PSNAME (PHASE(i))	phase of the i^{th} species
	MWSPEC(i)	molecular weight of i^{th} species; computed as: ΣFORMULA(j,i)*MWELEM(j), where FORMULA(j,i) is the stoichiometric number of j^{th} element in the i^{th} species, MWELEM(j) is the molecular weight of the j^{th} element, index j runs through all elements, and index i runs through all species
	MU0FORM(i)	standard chemical potential of the i^{th} species

1443-1558		table showing relationship of species to elements
	i,NAMES(i)	number and name of i^{th} chemical species
	FORMULA(j,i), j=1,ttlelem	stoichiometric number of each element in the i^{th} species

7.4 Standard RHOMIN Input File

The input file RHOMIN, another data base file, contains mineral densities. The RHOMIN file is required for titrate problems. It is not used for batch problems. RHOMIN contains the density of each of the solid species or minerals in the CHEMDAT file.

The RHOMIN input file, HMW_NP_AM_RTEST.RHOMIN, contains mineral densities in units of kg/m^3 or equivalently in g/L, $\rho_{MINERALS}$, for all of the minerals contained in the CHEMDAT file. The numerical values for mineral densities were taken from Weast (1980) when available, otherwise the minerals were arbitrarily assigned a value of 2000 g/L. Mineral densities are not needed to calculate the chemical equilibrium problems that FMT 2.3 solves. However, they were needed for transport calculations that explicitly accounted for the volumes of solid phases and the changes in porosity caused by mineral dissolution and precipitation, a feature incorporated in earlier versions of FMT (Novak, 1994) that is no longer supported. The only place this information is used within FMT 2.3 is in calculating the volumes of the initial "Erlenmeyer" solution for titrate problems. Thus, the particulars of titrate problems may be different if mineral densities in RHOMIN are altered. The RHOMIN file is an atavism that will be removed in the next major update of FMT.

Changing the values in RHOMIN will change the aqueous volume to solid volume ratio, which will change the response of the Erlenmeyer solution to the titrant volume. The titration curve will not change, but the points used to plot the titration curve will change.

*****WARNING*****
The user should not and is not expected to change the RHOMIN file.

In Table 12, which describes the input parameters for HMW_NP_AM_RTEST.RHOMIN, the "Variable Name" column is for the FMT program variables. FMT reads only the number on

each line of HMW_NP_AM_RTEST.RHOMIN. The species name on the line is for human readability and is not read by FMT.

Table 12. RHOMIN Input Parameters (See Appendix K for listing.)

Line	Variable Name	Description
1-66	RHOSPEC(i)	density of the i^{th} mineral species

8.0 ERROR MESSAGES

FMT has three types of messages—fatal error messages, warning messages, and informational messages. A system error message pertaining to divide by zero that may occur is also described after the section on fatal error messages.

In Table 13 all FMT messages are listed alphabetically with the type of message and a brief description. More detailed explanations are given in Sections 8.1 through 8.4.

Table 13. FMT Messages

Abbreviated Message	Message Type	Brief Explanation
AQ vio ...	Informational	Next iteration of the equilibrium calculations will include this aqueous species
BATCH CALCULATION ERRORS ...	Warning	Change between the initial and final elemental abundances greater than $\|10^{-6}\|$
CANNOT FIND LOCATION ...	Warning	CHEMDAT file does not have a "H+" species
"Charge" abundance is not ...	Fatal	INPUT file has a nonzero charge value
check problem type ...	Fatal	INPUT file does not contain the words BATCH or TITRATE where expected
divide by zero	Fatal	System error caused by insufficient water in the INGUESS file
DONT HAVE ANY REACTIONS ...	Informational	Equilibrium calculations generated a set of species that have a concentration value and can not react chemically among themselves
End of Autotitration Problem	Normal Run	Normal termination for a titration problem
ERROR IN INITIAL ESTIMATE ...	Fatal	Linear programming algorithm did not converge to produce an initial set of values for the root finding algorithm
"EXACT" mole amounts ...	Warning	Solution specified in the INGUESS file is not charge neutral
INPUT ERROR to ...	Fatal	Linear programming algorithm not coded correctly

MASS BALANCE ERRORS ...	Warning	Change between the initial and final elemental abundances greater than $\|10^{-6}\|$
MAXELEM= ...	Fatal	CHEMDAT file contains more elements than allowed
MAXSPEC= ...	Fatal	CHEMDAT file contains more elements and species than allowed
MUST PUT ALL AQUEOUS ...	Fatal	CHEMDAT file has aqueous species after solid species
MU(ttl)= ...	Informational	Equilibrium calculation has not converged after MAXIT iterations, indicating that one or more reactions are not at equilibrium
Negative Element or Species Abundance ...	Fatal	INPUT file has a negative value for an element or INGUESS file has a negative value for a species
"NEW T" option ...	Fatal	CHEMDAT file contains the word "NEW T"
No Convergence on Equi ...	Fatal	Equilibrium root finding algorithm did not converge
PROBLEM TOO LARGE ...	Fatal	INPUT file has too many beakers for a titration problem
Species "H2O" must be first ...	Fatal	CHEMDAT file does not have "H2O ..." at the beginning of all species
SINGLE BATCH EQUILIBRATION COMPLETED	Normal Run	Normal termination for a batch problem
SOLUBILITY PRODUCT VIOLATION ...	Informational	Solubility product for a solid species exceeded (supersaturated) during an iteration of the equilibrium calculations
'a number' SOLUBILITY PRODUCT VIOLATIONS	Informational	A count of the number of supersaturated solids per iteration
Switching Routine Hung ...	Informational	A species with a very small concentration has been added and then deleted from the equilibrium calculations three times
To use TITRATE option ...	Fatal	INPUT file does not have one of these words: LINEAR, LOG10, or ASREAD that specifies the amount allocated to each beaker
Trying to shift reaction ...	Fatal	Error message from coding

VALID CHARGE BALANCE ELEMENT NOT ...	Fatal	CHEMDAT file has a negative or zero value for the variable RPLWCHG
Was expecting the "TITRATE"...	Fatal	INPUT file does not have the word TITRATE following the section of unused values

8.1 Fatal Error Messages

A normal FMT run will terminate with a message displayed at the user's screen of either "SINGLE BATCH EQUILIBRATION COMPLETED" or "End of Autotitration Problem" for a batch or titrate problem, respectively. Fatal errors terminate the execution of FMT abnormally. These errors are always printed on the user's screen and unit 6*, the default value of which is the user's screen. The same and/or additional messages may be printed in the OUTPUT file.

Each error can generate one or more messages as shown below between lines of asterisks. A bracketed line preceding messages indicates where messages are printed. A pair of single quotes enclosing a phrase starting with 'value ...' indicates that the run time value in FMT will be listed.

The errors are listed in alphabetic order as they appear on the screen.

8.1.1 Error: "Charge" abundance is not . . .

```
****************************************
[on unit 6]
"Charge" abundance is not numerically zero

[on screen]
"Charge" abundance is not numerically zero
or
"Charge" abundance is not numerically zero, INJECTED
or
"Charge" abundance is not numerically zero, INITIAL

[in OUTPUT file]
"Charge" abundance is not numerically zero
****************************************
```

This error occurs when the last elemental amount in the INPUT file is greater than a numeric zero, that is, plus or minus 1.0×10^{-13}. The last line printed to the screen differs for batch and titration problems. If the last word in the line following "numerically zero" states:

---

* By default, unit 6 is the user's screen. The user could define a file = 6. If unit 6 is the user's screen, the message sent to 6 is printed first, followed by the [on screen] messages.

- no word, it is a batch problem; the last line in element list does not have a zero charge specified
- "INJECTED" the first or titrant solution does not have a zero charge specified
- "INITIAL" the second or titrated solution does not have a zero charge specified.

To correct this problem, change the charge amount in the INPUT file to 0.0.

8.1.2 Error: check problem type . . .

```
****************************************
[on unit 6]
check problem type option:  BATCH or TITRATE

[on screen]
CHECK PROBLEM TYPE SPECIFICATIONS

[in OUTPUT file]
check problem type option:  BATCH or TITRATE
****************************************
```

On line 4 of the INPUT file (the CDUM1 variable), the character string must be exactly 'BATCH' or 'TITRATE'.

Check that all the characters in the word are capitalized and the word is immediately surrounded by a pair of the single quote character. No spaces, tabs, or unprintable characters are permitted in the word.

8.1.3 Error: ERROR IN INITIAL ESTIMATE . . .

```
****************************************
[on screen]
ERROR IN INITIAL ESTIMATE DETERMINATION, INITGES

[on unit 6]
LINEAR SYSTEM INCONSISTENT [or] NO SOLUTION IS FEASIBLE

[in OUTPUT file]
ERROR IN RESULTS OF FEASBL
Results of call to FEASBL, IER= 2 [or] Results of call to FEASBL, IER= 3
****************************************
```

The linear programming routine could not find a set of species concentrations that satisfies the material balance for the given input. The linear programming algorithm is the weakest part of the code. The input could still represent a physical problem, but it may be a difficult combination of input values for the optimizing algorithm to find a solution.

Set up the initial solution desired in the INGUESS file and force FMT to read INGUESS with the flags 'MOLES' 'EXACT' set in the INPUT file. Then develop and enter a set of species concentrations that sum to the desired element totals and is charge-neutral. This will bypass the linear programming algorithm.

8.1.4 Error: INPUT ERROR to . . .

```
****************************************
[on unit 6]
INPUT ERROR to FEASBL
NEQ.gt.IDIM .or. IDIMP1.lt.IDIM+1 [or] NEQ.ge.NVAR

[on screen]
ERROR IN INITIAL ESTIMATE DETERMINATION, INITGES

[in OUTPUT file]
ERROR IN RESULTS OF FEASBL
Results of call to FEASBL, IER= 1
****************************************
```

NEQ, the number of linear equations must be greater than the first dimension of the coefficient array or the dimensions of the working arrays must be greater than NEQ+1 [or] NEQ must be greater than the number of variables, NVAR.

Contact the code sponsors. This message indicates programming errors.

8.1.5 Error: MAXELEM= 'value for . . .

```
****************************************
[on unit 6]
MAXELEM= 'value for MAXELEM'
TTLELEM= 'value for TTLELEM
Parameter Dimensions Too Small for this Problem
Must Increase MAXELEM to   MAXELEM='value for TTLELEM+1'

[on screen]
MAXELEM DIMENSION IS TOO SMALL
****************************************
```

This error occurs when the number of elements in the CHEMDAT file exceeds MAXELEM, a programmatic value which is set to 30.

Contact the code sponsors to set a higher limit for MAXELEM. If running FMT outside of WIPP, change the value set for parameter MAXELEM and recompile the code.

8.1.6 Error: MAXSPEC= 'value for . . .

```
****************************************
[on unit 6]
MAXSPEC= 'value for MAXSPEC'
```

```
TTLELEM= 'value for TTLELEM'
TTLSPEC= 'value for  TTLSPEC'
Parameter Dimensions Too Small for this Problem'
Must Increase MAXSPEC to   MAXSPEC= 'value for TTLELEM+TTLSPEC'

[on screen]
MAXSPEC DIMENSION IS TOO SMALL
**************************************
```

This error occurs when the number of species plus the number of elements in the CHEMDAT file exceeds MAXSPEC, a programmatic value which is set to 250.

Contact the code sponsors to set a higher limit for MAXSPEC. If running FMT outside of WIPP, change the value set for parameter MAXSPEC and compile the code.

8.1.7 Error: MUST PUT ALL AQUEOUS . . .

```
**************************************
[on screen]
MUST PUT ALL AQUEOUS SPECIES BEFORE MINERALS

[in OUTPUT file]
MUST PUT ALL AQUEOUS SPECIES BEFORE MINERALS
**************************************
```

This error occurs in the CHEMDAT file when a solid phase species is listed before an aqueous phase species.

In the CHEMDAT file, ensure that all aqueous species are declared before solid species.

8.1.8 Error: Negative Element or Species Abundance . . .

```
**************************************
[on screen]
Negative Element Abundance Entered
  or
Negative Species Abundance Entered

[in OUTPUT file for batch option]
Negative element abundance in input file
'element name'   'abund value'
STOPPING EXECUTION in ROUTINE ONEFLSH
  or
Negative species abundance in inguess file
'species name'   'abund value'
STOPPING EXECUTION in ROUTINE ONEFLSH

[in OUTPUT file for titration option]
Negative element abundance given, INJECTED
'element name'   'abund value'
STOPPING EXECUTION in ROUTINE FMT2P0
  or
Negative element abundance given, INITIAL
'element name'   'abund value'
STOPPING EXECUTION in ROUTINE FMT2P0
```

```
  or
Negative species abundance in inguess file
'species name'  'abund value'
STOPPING EXECUTION in ROUTINE FLASHIJ
**************************************
```

The error "Negative Element Abundance Entered" is generated when an element amount in the INPUT file is negative. The OUTPUT file contains the element name (from the CHEMDAT file) and the negative amount read from the INPUT file that caused this fatal error. For

- 'BATCH' problem: If the last line in the OUTPUT file states "ROUTINE ONEFLSH", the 'BATCH' flag was set in the INPUT file.

- 'TITRATE' problem: If the last line in the OUTPUT file states "ROUTINE FMT", the 'TITRATE' flag was set in the INPUT file. The first line of the error message "Negative element ..." in the OUTPUT file tells which solution the fatal error is in—the INJECTED solution is the first solution or titrant solution while the INITIAL is the second solution, or the titrated solution.

The related error "Negative Species Abundance Entered" is generated when a species amount in the INGUESS file is negative. The OUTPUT file contains the species name (from the CHEMDAT file) and the negative amount read from the INGUESS file that caused this fatal error. For

- 'BATCH' problem: If the last line in the OUTPUT file states "ROUTINE ONEFLSH", the 'BATCH' flag was set in the INPUT file.

- 'TITRATE' problem: If the last line in the OUTPUT file states "ROUTINE FLASHIJ", the 'TITRATE' flag and the 'MOLES' 'EXACT' flags were set for either the titrant or titrated solution by the INPUT file

Change the negative amount in the INPUT or INGUESS file to zero or positive amount. Check the rest of the INPUT or INGUESS file for any negative amounts and change to zero or positive amounts.

8.1.9 Error: "NEW T" option . . .

```
**************************************
[on screen]
"NEW T" option for non 298.15K discontinued
**************************************
```

This error occurs in the CHEMDAT file when the character string 'NEW T' is set.

Change the character string to 'nNEW T' in CHEMDAT. The 'NEW T' feature is not supported in this release of FMT.

8.1.10 Error: No Convergence on Equi . . .

```
**************************************
[on screen]
No Convergence on Equi Solid Suite

[in OUTPUT file]
EXITED SOLID ITERATION LOOP, MAXIMUM REACHED
diagnostics, no solid convergence achieved
list of element abundances follows:
'value for ABUND(i)' 'values for ELNAMES(i)'
list of species abundances follows:
'value for NMOLES(i)' 'values for NAMES(i)'
**************************************
```

This error occurs when there is no convergence in the equilibrium root finding algorithm after 20 iterations. (The number 20 is hard coded in the program.)

Contact the code sponsors. The algorithm has checked at least 20 different sets of solids and found no equilibrium solution. Either the problem is unusually complex or the particular set of element abundances represents a condition for which no solution can be found. In more than nine years experience with this equilibrium algorithm, this error has never occurred. If this error occurs, try breaking the problem into pieces and approach the desired equilibrium systems stepwise instead of all at once.

8.1.11 Error: PROBLEM TOO LARGE FOR . . .

```
**************************************
[on screen]
PROBLEM TOO LARGE FOR SPATIAL ARRAY DIMENSIONS

[in OUTPUT file]
TOO MANY NODES IN THE X AND Y DIRECTION
  NSPACE set to          'value for NSPACE'
  MWIDTH set to          'value for MWIDTH'
  MUST CONFORM TO THE FOLLOWING
  NSPACE .LE.            'value for MXSPACE'
  MWIDTH .LE.            'value for MXWIDTH'
  MWIDTH*NSPACE+2 .LE.  'value for MXANDY'
```

```
****************************************
```

This error appears in titrate problems when NSPACE, the number of Erlenmeyer solutions, is greater than 66.

Reduce the NSPACE parameter in the INPUT file to 66 or less and adjust the ASREAD volumes to 66 or less if using 'ASREAD.'

8.1.12 Error: Species "H2O" must be first . . .

```
****************************************
[on unit 6]
Species "H2O" must be first species in list
  Also, the first 3 chars. must be "H2O"

[on screen]
FIRST SPECIES NAME IS NOT H2O
****************************************
```

This error occurs in CHEMDAT when the variable NAME(1) does not contain the character string H2O as the first 3 characters. The NAME variable is read on line 14 as printed in the listing of HMW_NP_AM_RTEST.CHEMDAT (Appendix I).

Check that there are no spaces in the string H2O and that the string immediately follows the single quote mark.

8.1.13 Error: To use TITRATE option . . .

```
****************************************
[on unit 6]
To use TITRATE option, specify:
      'TITRATE' 'LINEAR or LOG10' DVMIN DVMAX
  where DVMIN and DVMAX are the minimum and maximum titrant volumes.
  When LINEAR is used, multiples of DVMIN (mL) are added to each beaker.
  When LOG10 is used, volumes from DVMIN (mL) to DVMAX (mL) are added to
    each beaker on a logarithmic scale.

[on screen]
Check Specifications for TITRATE Option

[in OUTPUT file]
To use TITRATE option, specify:
      'TITRATE' 'LINEAR or LOG10' DVMIN DVMAX
  where DVMIN and DVMAX are the minimum and maximum titrant volumes.
  When LINEAR is used, multiples of DVMIN (mL) are added to each beaker.
  When LOG10 is used, volumes from DVMIN (mL) to DVMAX (mL) are added to
    each beaker on a logarithmic scale.
****************************************
```

This error occurs when the INPUT file does not contain the one of the strings 'LINEAR', 'LOG10', or 'ASREAD' following the required 'TITRATE' string after the section of unused values (see line 100 in Table 6).

Check that one of the permissible character strings LINEAR, LOG10, or ASREAD is enclosed in single quotes and listed after the TITRATE string in the line.

8.1.14 Error: Trying to shift reaction . . .

```
****************************************
[in OUTPUT file]
Trying to shift reaction to the left, but
   SMLPRD is .LE. 0.d0

[or]
Trying to shift reaction to the right, but
   SMLRCT is .LE. 0.d0
****************************************
```

FMT is attempting to eliminate one of the species involved in a solids-only reaction but there is no more product (top message) or there are no more reactants (bottom message).

This is an error message left from code development. Contact the code sponsor if this error is triggered; however, we expect that this error will not occur.

8.1.15 Error: VALID CHARGE BALANCE ELEMENT NOT . . .

```
****************************************
[on screen]
VALID CHARGE BALANCE ELEMENT NOT SPECIFIED

[in OUTPUT file]
Need to specify the charge balance element
****************************************
```

This error occurs in the CHEMDAT file when the variable RPLWCHG is negative or zero. The RPLWCHG variable is read on line 866 as a 2 (the element Oxygen) in the listing of HMW_NP_AM_RTEST.CHEMDAT (Appendix I).

8.1.16 Error: Was expecting the "TITRATE" . . .

```
****************************************
[on unit 6]
Was expecting the "TITRATE" flag

To use TITRATE option, specify:
      'TITRATE' 'LINEAR or LOG10' DVMIN DVMAX
  where DVMIN and DVMAX are the minimum and maximum titrant volumes.
  When LINEAR is used, multiples of DVMIN (mL) are added to each beaker.
  When LOG10 is used, volumes from DVMIN (mL) to DVMAX (mL) are added to
```

```
    each beaker on a logarithmic scale.

[on screen]
second TITRATE flag incorrectly specified

[in OUTPUT file]
To use TITRATE option, specify:
      'TITRATE' 'LINEAR or LOG10' DVMIN DVMAX
  where DVMIN and DVMAX are the minimum and maximum titrant volumes.
  When LINEAR is used, multiples of DVMIN (mL) are added to each beaker.
  When LOG10 is used, volumes from DVMIN (mL) to DVMAX (mL) are added to
    each beaker on a logarithmic scale.
****************************************
```

This error occurs when the INPUT file does not contain the 'TITRATE' string after the section of unused values. (See INPUT file description for titrate problems, line 100 in Table 6.)

Check that the character string TITRATE is enclosed in single quotes and listed first in the line. There could also be missing lines or values prior to this line. In the unused values section, the variables and their permissible values must be present.

8.2 System Error Messages

There is one system error message "divide by zero" that occurs because of insufficient water in the INGUESS file to support the chemical reactions. When this occurs, the solvent H_2O has been consumed in the chemical reactions, so that when the amount of water (which is now zero) is used in the denominator of a divide operation, a "divide by zero" system error results, halting FMT execution. The FOR088 file was not generated due to the abnormal termination. The chemical system may be too complicated to solve as specified. Breaking the system into pieces and using the INGUESS file may help.

8.3 Warning Messages

There are warning messages that indicate the calculated results are not valid.

One or more messages are shown between lines of asterisks. A bracket line preceding any messages indicates where messages are printed. A pair of single quotes enclosing a phrase indicate that the run time value in FMT will be listed.

The errors are listed in alphabetic order as they appear on the screen.

8.3.1 Warning: BATCH CALCULATION ERRORS . . .

```
****************************************
[on unit 6]
```

```
BATCH CALCULATION ERRORS, L2 norm 'value for L2 norm'
SEE OUTPUT FOR MASS BALANCE ERROR INSTRUCTIONS

[in OUTPUT file]
BATCH CALCULATION ERRORS, L2 norm 'value for L2 norm'
(a listing of the initial and final abundances, element names and the absolute
value of the differences between the initial and final abundances)
MASS BALANCE ERROR INSTRUCTIONS
1) Check to see how much abundances have changed
   Should only happen in batch problems, or when
   flashing initial or injected conditions

2) This problem occurs when the diagnostic
   "Trying to get Internal Initial Guess"
   has been printed, and means that the initial
   guess provided by /MOLES/ is inadequate

3) Try flashing with /nMOLES/-- this is the
   easiest way to try to fix the problem
**************************************
```

This message warns that material balance errors are present during the flash calculation. This message occurs when element abundances, including charge, change by more than 10^{-6} (relative or absolute depending on totals) during an equilibration. FMT prints the above message and continues on to the next flash in a titration problem.

When this error is triggered, it usually means that modifications to the CHEMDAT file were made incorrectly.

8.3.2 Warning: CANNOT FIND LOCATION OF . . .

```
**************************************
[on unit 6]
CANNOT FIND LOCATION OF "H+" INVALIDATING pH VALUE

[in OUTPUT file]
CANNOT FIND LOCATION OF "H+" INVALIDATING pH VALUE
**************************************
```

This message occurs in the CHEMDAT file when the exact species name of 'H+' is missing from the species list or a space or unprintable character precedes the H+. The only effect of this warning is that pH and pmH values will not be printed. This warning occurs if the H+ species is renamed such that the first 2 characters are not H+.

8.3.3 Warning: "EXACT" mole amounts . . .

```
**************************************
[in OUTPUT file]
"EXACT" mole amounts not charge balanced
   CHARGE= 'value of charge ABUND'
**************************************
```

FMT has calculated the elemental abundances using the mole amounts given in the INGUESS file. The solution must be charge neutral otherwise FMT will modify the abundance. This error occurs when the species amounts in the INGUESS file do not maintain charge neutrality. The absolute value of the charge must equal or exceed 1.0×10^{-12} for this error to occur.

Check the species amounts in the INGUESS file, being sure to maintain charge neutrality. For example, if you are increasing the amount of a positively charged species, then add the necessary amount of a negatively charged species, observing stoichiometric rules.

8.3.4 Warning: MASS BALANCE ERRORS . . .

```
**************************************
[on unit 6]
MASS BALANCE ERRORS at ISPACE= 'value of Erlenmeyer solution'
**************************************
```

See explanation in Section 8.3.1.

8.4 Informational Messages

There are informational messages that indicate where the code is during execution or what it is doing. These messages, presented in alphabetical order, are described below.

8.4.1 AQ vio 'value of mu' . . .

```
**************************************
[in OUTPUT file]
AQ  vio 'value of mu'  'species name' 'name index number'
**************************************
```

This message indicates that an aqueous species is not at equilibrium, and that it will be included in the next round of equilibration calculations. The message is triggered when the species activity is calculated to be greater than MINABU x 10^{-6} (usually 10^{-24}).

8.4.2 DONT HAVE ANY REACTIONS . . .

```
**************************************
[on unit 6]
 ***********************************************
 ***********************************************
 **** DONT HAVE ANY REACTIONS TO EQUILIBRATE ***
 ****** BUT CONTINUING CALCULATION ANYWAY ******
 ***********************************************
 ***********************************************

[in OUTPUT file]
```

```
**********************************************
**********************************************
**** DONT HAVE ANY REACTIONS TO EQUILIBRATE ***
****** BUT CONTINUING CALCULATION ANYWAY ******
**********************************************
**********************************************
**************************************
```

This message occurs when there are no possible chemical reactions among the species with nonzero concentrations. This can occur during the normal process of solving the equilibrium system.

8.4.3 MU(ttl)= 'value of mu' . . .

```
**************************************
[on unit 6]
MU(ttl)= 'value of mu' x 'value of Erlenmeyer solution'

[in OUTPUT file]
nonconvergent elemental abundances
MU(ttl)= 'value of mu' x 'value of Erlenmeyer solution'
table of element abundance
'value for abund(i)' 'value for elnames(i)'
**************************************
```

This is not a fatal error, but it is more than a run-time message. This message occurs when one or more reactions are not at equilibrium after MAXIT iterations. MAXIT is the number of iterations for minimizing free energy and set by the CHEMDAT file. The output from the runs in which this message occurs must be checked carefully by the user to see if they are suitable to use. Often this message occurs at intermediate stages on the approach to the equilibrium composition, and final results are at equilibrium.

8.4.4 SOLUBILITY PRODUCT VIOLATION . . .

```
**************************************
[on unit 6]
 ************SOLUBILITY PRODUCT VIOLATION*************
'species name' ** 'value of mu'  **

[in OUTPUT file]
 ************SOLUBILITY PRODUCT VIOLATION*************
'species name' ** 'value of mu'  **
**************************************
```

This message occurs during execution of a batch problem when the solubility product of a mineral is exceeded. This message refers to FMT's normal algorithmic attempts to find the equilibrium suite of solid phases.

8.4.5 'count of ' Solubility Product Violations . . .

```
**************************************
```

```
[on unit 6]
'count of ' Solubility Product Violations
 Adding solid 'name of solid species most oversaturated'

[in OUTPUT file]
'count of ' Solubility Product Violations
 Adding solid 'name of solid species most oversaturated'
**************************************
```

This message occurs during execution of a batch problem whenever one or more solid species are supersaturated. The solid that is calculated to be the most supersaturated will be included in the next round of equlibrium calculations.

8.4.6 Switching Routine Hung . . .

```
**************************************
[on unit 6]
Switching Routine Hung, Ending Batch #:    'beaker number of Erlenmeyer solution'
**************************************
```

A species has a calculated concentration right on the boundary between existing and not existing (MINABU value multiplied by 1.0×10^{-6}) and FMT cannot decide whether to include it or not. This message is triggered when FMT adds the same species three times in a row but the species gets deleted in the equilibrium root finding algorithm. Because the boundary between "existing" and "not existing" is very low (1.0×10^{-24}, about 1 moiety per kg H_2O), this message has no consequences.

9.0 DESCRIPTION OF OUTPUT FILES

FMT generates a primary OUTPUT (.OUT) file and the secondary output files as shown in Figures 1 and 2 in Section 6.1. Secondary output files vary according to whether a batch (single flash) calculation or titrate (multiple flash) calculation is performed. (A batch problem has one flash calculation. A titrate problem has a user-specified number of flash calculations.) FOR088 is the secondary file for batch problems; TITRATE is the secondary file for titrate problems.

9.1 OUTPUT

For both batch and titration calculations, the primary file OUTPUT (.OUT) file lists the problem identity, echoes the CHEMDAT file, and contains a summary of element concentrations, species concentrations, and equilibrium parameters for each flash calculation performed.

Note that while the user is printing the OUTPUT file, page breaks will occur. The listings appended to this guide do not emulate the page break as a separate page but show such a line as a Fortran page break, i.e., the line is prefixed with the character "1."

9.1.1 Batch Problem

Table 14 explains the OUTPUT (.OUT) file generated from a batch problem called BATCH_DOC. The "Line" column refers to the line numbers listed in BATCH_DOC.OUT. "Variable Name" column shows applicable FMT program variables and some formulas.

Table 14. OUTPUT File Description for Batch (See Appendix L for sample listing.)

Line	Variable Name	Description
1	INFNM	INPUT file name
2	INGFNM	INGUESS file name
3	OUFNM	OUTPUT file name
4	CHFNM	CHEMDAT file name
5		notation; FMT sets temperature to 298.15 Kelvin
6	TITLE99	problem title specified on line 1 of INPUT file with 'FMT' and version number appended
7-8	DBASE1, DBASE2	unique data base identification specified on lines 1 and 2 of CHEMDAT file
10-13		this location would normally be filled with an echo print of ion interaction parameters and chemical species definitions, as read from the CHEMDAT input file (Appendix I). This information is reproduced in the OUTPUT file listing in Appendix J and is described in Section 7.3.
15-27		this section contains computation status indicators printed during calculations to find the equilibrium system
21-24	NAMES(i), MU(i)	at the end of the first convergence loop, the solids brucite and magnesium oxychloride "MgOxychloride," were oversaturated, and thus the system was not at equilibrium
26	NKSPVIO	number of solubility product violations for solids (minerals)
27	NAMES(i)	postulated that brucite was present in the equilibrium system, and thus added to the equilibrium calculations
28	ALLITER	number of times the diagonalized Hessian matrix system of equations was solved to reach the calculated equilibrium state
29		Note: a page break occurs; the first character "1" indicates a Fortran page break and is deleted before printing the remaining line
29-31	TITLE99, DBASE1, DBASE2	problem title and CHEMDAT input file (Appendix I) identification

32	PRESSUR, TEMPERA	pressure and temperature for batch problem
34-61		table of Elemental Abundances
	ABUND(i)	"Total Moles" column contains the exact number of moles for each element as read from the INPUT file, or as calculated from species abundances as read from the INGUESS file
	AQMOLES(i)/ KGH2O	"Aq. Molality" column is the total molality for each element in the aqueous phase
	AQMOLES(i)/ SOLNVOL	"Aq. Molarity" column is the total molarity for each element in the aqueous phase. This number is calculated from the solution density, as discussed in this table on lines 63-76.
	AQMOLES(i)/ SOLNVOL× MWELEM(i) ×1000	"Aq. mg/liter" column is the total aqueous element concentration in milligrams per liter
	ELNAMES(i)	identifies the element name corresponding to the row of values in the table
63-76		this section documents the calculation of solution density, a quantity that is required only for converting molal units to Molar units. In batch problems, the density is used only to produce the volume based concentration units (Molar, mg/liter) printed in the OUTPUT file. The actual calculation of equilibrium is conducted using mass-based, i.e., molal, units. FMT uses a correlation based on NaCl solutions (as noted on line 38) to calculate solution density from total dissolved solids (TDS).
64-66	SOLMASS, KGH2O×1000, TDSGPKG	values calculated from equilibrium compositions
69	SPRHO	density specified in the INPUT file for titrate problems. For BATCH problems the solution density from the NaCl correlation is automatically used.
72-73	SOLNVOL, TDS	calculated values based on specified density on line 69
75	DENSITY(2, TDSGPKG)	density calculated by FMT using the NaCl correlation
76	(DENSITY(2, TDSGPKG)/ SPRHO-1.)×100	difference between the specified density (line 69) and the density calculated by FMT which will always be zero for BATCH problems

80-164		table listing detailed information about the species in the equilibrium problem. Note that only species that can be formed from elements with nonzero concentrations are included. Species are sorted approximately in order of decreasing concentration. For example, the total phosphorus element concentration on line 59 is zero, so no detailed information is given for phosphorus species.
	NAMES(i)	"Species Name" column
	MOLALTY(i) or for solids: NMOLES(i)/ NMOLES(1)/ MWH2O	"Molality" column contains the species molality, moles per kg H_2O, for all species including solids. However, the entry for water is not molality of water, which is invariant, but the mole fraction H_2O in the aqueous phase, as noted on line 173.
	LNGAMA(i)× MOLALTY(i)	"Activity" column is the product of the "Molality" and "Act Coef" columns or is defined to be 1 for solids
	LNGAMA(i) or 1.0 for solids	"Act Coef" column is the calculated activity coefficient for the species, which is 1 by definition for solids
	NMOLES(i)	"Total Moles" column is the total number of moles for the i^{th} species
	NMOLES(i)/ SOLNVOL	"Molarity" column is the volume-based concentrations calculated from the "Molality" column using the solution density described above on lines 63-76
	NMOLES(i)/ SOLNVOL× MWSPEC(i)× 1000	"mg/liter" is the volume-based concentrations calculated from the "Molality" column
	MU(i)/LN10	"descriptor" column has various meanings, as stated in the notes on lines 175-179
166	PHVECT	pH: the negative base 10 logarithm of hydrogen ion activity
	-(NMOLES (NPROTON)/ NMOLES(1)/ MWH2O)	pmH: the negative base 10 logarithm of hydrogen ion molality
167	OSM	osmotic coefficient, a value related to the activity of water; a value calculated from the Pitzer equations
168	LNGAMA(1)×100	equilibrium relative humidity, equal to 100% times the water activity

169	IONICST	ionic strength, in molal units, defined as $\sum_{i=2}^{Nspec} z_i^2 m_i$, where z_i is the charge on the i^{th} species, m_i is the molality of the i^{th} species, and index i runs from species 2 through all aqueous species, with species 1 defined as H_2O
170	SPRHO	solution density, calculated as described on lines 63-76
171		fugacity and log of fugacity of $CO_2(g)$ (see derivation in Appendix U)
173-174		notes defining water and gas molality
175-179		notes describing the descriptor column in table of concentrations for batch system
181	ΣCHEMPOT(i)× NMOLES(i)	the total dimensionless Gibbs free energy for the solution; the quantity that is minimized to find the equilibrium composition
183	NINVERS	total number of times the diagonalized Hessian matrix system of equations was solved; for batch problem, this value is the same as ALLITER on line 28
184	ICNT	number of times the species list was changed for computational purposes in the minimization algorithm

In the BATCH_DOC.OUT file on lines 34-61, the first table in the file gives the elemental abundances in various units. The first column "Total Moles" provides the basis for computation, i.e., the amount of each element, independent of phase, including hydrogen and oxygen. It is convenient to specify material on an approximately 1 kg H_2O basis (~55.5 moles H_2O). The second column "Aq. Molality" (Aq. means aqueous) gives the aqueous phase totals; it is this portion of the output that corresponds to the aqueous phase element totals listed above. The "Aq. Molarity" and "Aq. mg/liter" columns are provided for the convenience of those users who prefer these units. However, these units depend on the value used for solution density, which is approximated by FMT from a correlation based on the density of NaCl solutions. "Aq." means aqueous.

The second table, Table of Concentrations for Batch System, on lines 80-164 lists molality, activity, activity coefficient, and a descriptor for each chemical species that can be made from the elements with nonzero concentrations. For example, note that there are no species containing

"Air", "TracerEl", "Th(IV)", etc. in this list. These species are sorted in approximate order of decreasing molality.

The descriptor serves several functions. First, it is the value that is actually tested for convergence (note that all values of the descriptor are less than the 10^{-6} as specified in line 7 of the output file listing for the CHEMDAT file; see Appendix J). The *component* species, lines 84-93, do not have descriptors because these are species from which all other species are formed by chemical reaction. (This quickly leads into an arcane discussion of the algorithm used to calculate equilibrium. The interested user should refer to Smith and Missen (1991), particularly Chapter 6.) The descriptor values given for noncomponent species, lines 94-104, all have absolute values less than 10^{-6}, thus indicating convergence. The remaining species, lines 105-164, all have zero concentration. Most of these species are solids, and the descriptor is the saturation index, $SI=\log_{10}(Q/K_{sp})$, an indication of how saturated the solution is with respect to that solid. A saturation index of 0.0 indicates the solution is exactly saturated. A saturation index less than zero indicates undersaturation. FMT does not allow solutions to be oversaturated.

Lines 157-158 show that the species NaOH(aq) and HCl(aq) have zero concentrations, and descriptors of –293 and –254 respectively. As the note in line 178 indicates, the descriptor value for aqueous species with zero concentrations is approximately equal to the $\log_{10}$ concentration of that aqueous species in this solution. (For comparison, one atom in 1 kg H_2O would have a molal concentration of 1.6×10^{-24} molal, corresponding to a descriptor value of –23.8.) These values are a consequence of the choice of values for the standard chemical potentials of these species. As discussed in the CHEMDAT data base documentation (Section 7.3.3), these species are nonphysical and included for convenience only.

9.1.2 Titrate Problem

Table 15 explains the printout for a titrate problem using the OUTPUT file generated from executing Np_NaCl_BM_LOG, Np_NaCL_BM_LIN and Np_NaCl_BM. The "Line" column refers to the line numbers listed in Np_NaCl_BM_LOG.OUT. "Variable Names" column shows FMT's program names and some formulas.

Table 15. OUTPUT File Description for Titrate (See Appendices M, N, and O for sample listings of Np_NaCl_BM_LOG.OUT, Np_NaCl_BM_LIN.OUT, and Np_NaCl_BM.OUT, respectively.)

Line	Variable Name	Description
1	INFNM	INPUT file name
2	INGFNM	INGUESS file name
3	OUFNM	OUTPUT file name
4	CHFNM	CHEMDAT file name
5		notation that temperature is set to 298.15 Kelvin by FMT
6	TITLE99	problem title specified on line 1 of INPUT file with 'FMT' and version number appended
7-8	DBASE1, DBASE2	unique data base identification specified on lines 1 and 2 of CHEMDAT file
10-309		most information in lines 10-309 corresponds to the OUTPUT file listing of the CHEMDAT portion as provided in Appendix J and is described therein
10-12		repeat of lines 7-9 in OUTPUT file for CHEMDAT (Appendix J)
14		notation, user selects data base not to echo in OUTPUT file
16-33		repeat of lines 12-29 in OUTPUT file for CHEMDAT (Appendix J)
36-37		repeat of lines 1285-1286 in OUTPUT file for CHEMDAT (Appendix J)
40		notation, FMT has a titration problem
43-309		repeat of lines 1293-1559 in OUTPUT file for CHEMDAT (Appendix J)
311	RHFNM	RHOMIN file name
312-405		summary information for the titrant solution flash calculation
406-503		summary information for the Erlenmeyer solution flash calculation

504		notation; first beaker of Erlenmeyer solution
505-602		summary information for the first beaker (same as Erlenmeyer solution when corrected for different volumes)
603		notation; second beaker of Erlenmeyer solution
604-701		summary information for addition of DV(2) to 1 liter of the Erlenmeyer solution
702		notation; third beaker of Erlenmeyer solution
703-800		summary information for addition of DV(3) to 1 liter of the Erlenmeyer solution
801		notation; fourth beaker of Erlenmeyer solution
802-899		summary information for addition of DV(4) to 1 liter of the Erlenmeyer solution
900		notation; fifth beaker of Erlenmeyer solution
901-998		summary information for addition of DV(5) to 1 liter of the Erlenmeyer solution
999		notation; sixth beaker of Erlenmeyer solution
1000-1097		summary information for addition of DV(6) to 1 liter of the Erlenmeyer solution
1098		notation; seventh beaker of Erlenmeyer solution
1099-1196		summary information for addition of DV(7) to 1 liter of the Erlenmeyer solution
1197		notation; eighth beaker of Erlenmeyer solution
1198-1295		summary information for addition of DV(8) to 1 liter of the Erlenmeyer solution
1296		notation; ninth beaker of Erlenmeyer solution
1297-1394		summary information for addition of DV(9) to 1 liter of the Erlenmeyer solution
1395		notation; tenth beaker of Erlenmeyer solution

1396-1493		summary information for addition of DV(10) to 1 liter of the Erlenmeyer solution
1494		notation; eleventh beaker of Erlenmeyer solution
1495-1592		summary information for addition of DV(11) to 1 liter of the Erlenmeyer solution
1593		notation; twelfth beaker of Erlenmeyer solution
1594-1691		summary information for addition of DV(12) to 1 liter of the Erlenmeyer solution
1692		notation; thirteenth beaker of Erlenmeyer solution
1693-1790		summary information for addition of DV(13) to 1 liter of the Erlenmeyer solution
1791		notation; fourteenth beaker of Erlenmeyer solution
1792-1889		summary information for addition of DV(14) to 1 liter of the Erlenmeyer solution
1890		notation; fifteenth (last) beaker of Erlenmeyer solution
1891-1988		summary information for addition of DV(15) to 1 liter of the Erlenmeyer solution
1989	TIFNM	TITRATE file name

9.2 FOR088

The batch-generated secondary file FOR088 contains three columns from the "Table of Concentration for Batch System" in the OUTPUT file. The columns are total species moles, species name, and species molality with the species reordered as listed in the CHEMDAT file. FOR088 and the input file INGUESS have the same format, and are designed to facilitate creation of a specific solution composition. FOR088 can be renamed and used as a template for an INGUESS file which the user can edit. Table 16 explains the FOR088 file generated from a batch problem. The "Line" column refers to the line numbers listed in BATCH_DOC.FOR088.

Table 16. FOR088 File Description for Batch (See Appendix P for sample listing.)

Line	Variable Name	Description
1-115	NMOLES(i)/ NMOLES(1)/ MWH2O where NMOLES(2) same as NMOLES(H_2O)	moles of the i^{th} species normalized to 1 kg H_2O (numerically equivalent to molality) $\left[\frac{\text{nmoles(i)}}{\text{nmoles}(H_2O) * \text{mw}H_2O}\right] * 1\text{kg}\,H_2O$
	NAMES(i)	the i^{th} species names
	NMOLES(i)	total number of moles for the i^{th} species

9.3 TITRATE

The TITRATE file, a secondary output file for the titrate problem, contains the titrant volumes and the equilibrated concentrations of all species, and the pH and ionic strength of each flash calculation from the OUTPUT file. The concentrations from each flash calculation have been reorganized by species for easy transfer to a graphics program for plotting.

Table 17 describes a TITRATE file generated by FMT. The "Line" column refers to the line numbers listed in Np_NaCl_BM_LOG.TITRATE. Np_NaCl_BM_LIN.TITRATE and Np_NaCl_BM_LIN.TITRATE have similar sample listings in Appendices R and S, respectively.

Table 17. TITRATE File Description (Appendix Q)

Line	Variable Name	Description
1-3	TITLE99, DBASE1, DBASE2	problem title and CHEMDAT identification
5-20	j, DV(j)*1.d3	j^{th} beaker and titrant volume added to j^{th} beaker
23-245		table of all species molal concentrations
	NAMES(i)	up to nine columns of species names on a line

	j, SPMOLES(i,j)/ ACONST(i)	j^{th} beaker and species molal concentration
247-262	j, IONICST(J)	j^{th} beaker and ionic strength
	DV(j)*1.d3	titrant volume
	PHVECT	pH of solution
	-(NMOLES (NPROTON)/ NMOLES(1)/ MWH2O)	pmH: the negative base 10 logarithm of hydrogen ion molality

10.0 REFERENCES

Denbigh, K. 1981. *The Principles of Chemical Equilibrium.* Cambridge: Cambridge University Press.

Felmy, A.R., D. Rai, and R.W. Fulton. 1990. "The Solubility of $AmOHCO_3(c)$ and the Aqueous Thermodynamics of the System Na^+-Am^{3+}-HCO_3^--OH^--H_2O." *Radiochimica Acta* vol. 50: 193-240.

Felmy, A.R., D. Rai, J.A. Schramke, and J.L. Ryan. 1989. "The Solubility of Plutonium Hydroxide in Dilute Solution and in High-Ionic-Strength Chloride Brines." *Radiochimica Acta* vol. 48: 29-35.

Felmy, A.R., and J.H. Weare. 1986. "The Prediction of Borate Mineral Equilibria in Natural Waters: Application to Searles Lake, California." *Geochimica et Cosmochimica Acta* vol. 50: 2771-2783.

Harvie, C.E., N. Møller, and J.H. Weare. 1984. "The Prediction of Mineral Solubilities in Natural Waters: The Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O System to High Ionic Strength at 25_C." *Geochimica et Cosmochimica Acta* vol. 48: 723-751.

Harvie, C.E., and J.H. Weare. 1980. "The Prediction of Mineral Solubilities in Natural Waters: The Na-K-Mg-Ca-Cl-SO_4-H_2O System from Zero to High Concentration at 25°C." *Geochimica et Cosmochimica Acta* vol. 44: 981-997.

Moore, R.C. "Validation of data entries in computer data file HMW_NP_AM.CHEMDAT," memorandum to C.F. Novak. 20 March 1995. Copy on file at Sandia WIPP Central Files.

Neck, V., J.I. Kim, and B. Kanellakopulos. 1994. Thermodynamic Behavior of Neptunium(V) in Concentrated NaCl and $NaClO_4$ Solutions. translated from Thermodynamisches Verhalten von Neptunium(V) in konzentrierten NaCl- und $NaClO_4$ Lösungen. KfK 5301. Institut für Nukleare Entsorgungstechnik, Institut für Heiße Chemie, Kernforschungszentrum Karlsruhe.

Novak, C.F. 1995a. "Creation and Definition of the Data base for FMT called "HMW_NP_AM.CHEMDAT," version date 94.01.17." memorandum to N.J. Dhooge. 18 January 1995. Copy on file at Sandia WIPP Central Files.

Novak, C.F. 1995b. "Correction to the Data base for FMT called "HMW_NP_AM.CHEMDAT," to create version date 95.01.31." memorandum to N.J. Dhooge. 31 January 1995. Copy on file at Sandia WIPP Central Files.

Novak, C.F. 1995c. "Input/Output Files for FMT Version 1.2." memorandum to Sandra C. Babb and Chris C. Crafts. 13 February 1995. Copy on file at Sandia WIPP Central Files.

Novak, C.F. 1995d. "'BATCH' Benchmark Problem for FMT: WIPP SPC Brine." memorandum to Ellen S. Dombroski. 14 February 1995. Copy on file at Sandia WIPP Central Files.

Novak, C.F. 1995e. "Input/Output Files for 'TITRATE' Problems; Benchmark Problem for FMT: The Solubility of $NaNpO_2CO_3(s)$ in 5.61 molal NaCl as a Function of Carbonate Concentration." memorandum to Ellen S. Dombroski and Sandra C. Babb. 15 February 1995. Copy on file at Sandia WIPP Central Files.

Novak, C.F. 1995k. "Performing FMT Simulations with Fixed $CO_2(g)$ Fugacity ("Partial Pressure")." memorandum to Chris C. Crafts and Sandra C. Babb. 20 March 1995. Copy on file at Sandia WIPP Central Files.

Novak, C.F. 1994. "Development of the FMT Chemical Transport Simulator: Coupling Aqueous Density and Mineral Volume Fraction to Phase Composition." *Proceedings of the Fourth International Conference on the Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere* . Special Issue of Radiochimica Acta. R. Oldenbourg Verlag: München, Germany.

Novak, C.F., and K.E. Roberts. 1995. "Thermodynamic Modeling of Neptunium(V) Solubility in $Na\text{-}CO_3\text{-}HCO_3\text{-}Cl\text{-}ClO_4\text{-}H\text{-}OH\text{-}H_2O$ Electrolytes," *Materials Research Society Symposium*

Proceedings, Volume 353. International Symposium on the Scientific Basis for Nuclear Waste Management (18th: 1994: Kyoto, Japan). pp. 1119-1128.

Pitzer, K.S. 1991. "Ion Interaction Approach: Theory and Data Correlation," Chapter 3, in *Activity Coefficients in Electrolyte Solutions.* Boca Raton, Florida: CRC Press. pp. 75-153.

Pitzer, K.S. 1973. "Thermodynamics of electrolytes I: Theoretical basis and general equations." *J. Phys. Chem.* vol. 77, 268-277.

Pitzer, K.S., and L.F. Silvester. 1976. "Thermodynamics of Electrolytes. VI. Weak Electrolytes Including H_3PO_4." *Journal of Solution Chemistry* vol. 5: 269-278.

Pitzer, K.S., and L.F. Silvester. 1978. "Thermodynamics of Electrolytes. 11. Properties of 3:2, 4:2, and Other High-Valence Types." *Journal of Physical Chemistry* vol. 82: 1239-1242.

Rai, D., A.R. Felmy, and R.W. Fulton. 1994. "The Nd^{3+} and Am^{3+} Ion Interactions with SO_4^{2-} and their Influence on $NdPO_4$(c) Solubility." *Journal of Solution Chemistry.* submitted June 1994.

Rai, D., A.R. Felmy, and R.W. Fulton. 1992a. "Solubility and Ion Activity Product of $AmPO_4 \cdot xH_2O$(am)." *Radiochimica Acta* vol. 56: 7-14.

Rai, D., A.R. Felmy, R.W. Fulton, and J.L. Ryan. 1992b. "Aqueous Chemistry of Nd in Borosilicate-Glass/Water Systems." *Radiochimica Acta* vol. 58/59: 9-16.

Rai, D., R.G. Strickert, D.A. Moore, and J.L. Ryan. 1983. "Am(III) Hydrolysis Constants and Solubility of Am(III) Hydroxide." *Radiochimica Acta* vol. 33: 201-206.

Rao, L., D. Rai, A.R. Felmy, and RW. Fulton. 1994. "Solubility of $NaNd(CO_3)_2 \cdot 6H_2O$ in Concentrated Sodium Carbonate and Sodium Bicarbonate Solutions." *Radiochimica Acta* vol. 24, no. 2: 879-895.

Smith, W.R., and R.W. Missen. 1991. Chemical Reaction Equilibrium Analysis: Theory and Algorithms. New York: John Wiley and Sons.

Smith, J.M., and H.C. Van Ness. 1975. *Introduction to Chemical Engineering Thermodynamics*. New York: McGraw-Hill.

Wagman, D.D., W.H. Evans, V.B. Parker, R.H. Schumm, I. Halow, S.M. Bailey, K.L Churney, R.L. Nuttall. 1982. The NBS Tables of Chemical Thermodynamic Properties. Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units. *Journal of Physical and Chemical Reference Data* vol. 11, Supplement 2.

Weast, R.C. 1980. *CRC Handbook of Chemistry and Physics* 60th ed. Chemical Rubber Publishing Company, Boca Raton, Florida.

11.0 APPENDICES

Note

The numbers to the left of each line in Appendices A through T are not actually present in the files and screen displays; they are used solely to reference the lines in this guide.

Note

The sample files and displays provided in Appendices A through T are examples *only*. They *are not* necessarily representative of files used to support the WIPP PA regulatory calculation.

Appendix A: Sample Screen Display of BATCH_DOC

See Table 2 for explanation of this screen display.

```
Enter chemdat file name to search on: np_am
Enter rhomin file name to search on: np_am
Enter input file name (without .extension): batch_doc
%CMS-I-LIBIS, library is WP$NONPA_CMSROOT:[FMT]
%CMS-S-LIBSET, library set
-CMS-I-SUPERSEDE, library list superseded

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.CHEMDAT "Initial load"
FMT_HMW_NP_AM_960823.CHEMDAT "CHEMDAT DATABASE FILE FOR FMT 2.2 REGRESSION TESTING"
FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
FMT_HMW_NP_AM_RTEST.CHEMDAT "CHEMDAT DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING"
Select CHEMDAT name from list above: FMT_HMW_NP_AM_RTEST.CHEMDAT
Your CMS library list consists of:
    WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.RHOMIN "Initial load"
FMT_HMW_NP_AM_960823.RHOMIN "RHOMIN DATABASE FILE FOR FMT 2.2 REGRESSION TESTING"
FMT_HMW_NP_AM_RTEST.RHOMIN "RHOMIN DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING"
Select RHOMIN name from list above: FMT_HMW_NP_AM_RTEST.RHOMIN
Your CMS library list consists of:
    WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.RHOMIN fetched
Enter "Y" or "y" to echo database in OUT file: y

                  image name: "FMT_PA97"
                  image file identification: "P PA97 2.3"
                  image file build identification: ""
                  link date/time:  1-APR-1997 09:55:34.40
                  linker identification: "A11-14"

DG_BYPASS flag set to nDG_BYPASS
[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs                FMT V2.3
DATABASE:   HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31    Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

Accuracy of reactions is              1.0000E-06
Minimum elemental abundance is        1.0000E-18
Number of Aqueous Species is            50

ACTIVITY COEF. FLAG PITZACT
Finished do 10:  read b(0) b(1) b(2) cphi
Finished do 20:  read theta(c,c)
Finished do 30:  read theta(a,a)
Finished do 40:  read psi(c,c,a)
Finished do 50:  read psi(a,a,c)
Finished do 55:  read neucat(n,c)
Finished do 65:  read neuani(n,a)
Finished do 66:  read ptztsi(n,c,a)
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

Char Flags: FLOW/BATCH/TITRATE:  BATCH       UNUSED
this is a BATCH problem

Echo of Mole Specifications:  nMOLES     nEXACT
ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH
   110.222364000000       Hydrogen
   55.1654821000000       Oxygen
 0.200000000000000        Sodium
 1.000000000000000E-002   Potassium
 1.000000000000000E-003   Magnesium
 1.000000000000000E-004   Calcium
 0.110000000000000        Chlorine
 1.000000000000000E-003   Sulfur
 1.000000000000000E-004   Carbon
 0.000000000000000E+000   PosIon
 0.000000000000000E+000   NegIon
 0.000000000000000E+000   Air
 1.000000000000000E-007   Boron
 0.000000000000000E+000   Bromine
 0.000000000000000E+000   TracerEl
 0.000000000000000E+000   Th(IV)
 0.000000000000000E+000   Am(III)
 0.000000000000000E+000   U(VI)
 0.000000000000000E+000   Np(V)
 0.000000000000000E+000   ClO4-(EL)
```

Appendix A: Sample Screen Display of BATCH_DOC

```
 84  0.000000000000000E+000 Phosphorus
 85  0.000000000000000E+000 Electron
 86  4.906053920000000E-017 Charge
 87 .LT. (MINABU*1.d-6) moles NaBO2.NaCl.2H2O___Teepleite_(20_C); del&switch
 88 .LT. (MINABU*1.d-6) moles NaB5O8.5H2O_____Sodium_Pentaborate; del&switch
 89 .LT. (MINABU*1.d-6) moles NaOH(aq).....to.titrate.base.only; del&switch
 90 .LT. (MINABU*1.d-6) moles HCl(aq).......to.titrate.acid.only; del&switch
 91 .LT. (MINABU*1.d-6) moles K2B4O7.4H2O___K-Tetraborate_(30_C); del&reopt
 92 .LT. (MINABU*1.d-6) moles B4O5(OH)4=               B4O5(OH)4=; del&reopt
 93 .LT. (MINABU*1.d-6) moles K8H6(SO4)7_______________Misenite; del&reopt
 94 .LT. (MINABU*1.d-6) moles K8H4(CO3)6.3H2O___K-Sequicarbonate; del&switch
 95 .LT. (MINABU*1.d-6) moles B3O3(OH)4-               B3O3(OH)4-; del&switch
 96 .LT. (MINABU*1.d-6) moles Ca4Cl2(OH)6.13H2O__CaOxychloride A; del&switch
 97
 98 ************SOLUBILITY PRODUCT VIOLATION************
 99 ** Mg(OH)2_____________________Brucite **  1.00E+01 **
100
101 ************SOLUBILITY PRODUCT VIOLATION************
102 ** Mg2Cl(OH)3.4H2O______MgOxychloride **  6.69E+00 **
103
104           2 Solubility Product Violations
105 Adding solid Mg(OH)2_____________________Brucite
106 .LT. (MINABU*1.d-6) moles NaOH(aq).....to.titrate.base.only; del&switch
107 .LT. (MINABU*1.d-6) moles HCl(aq).......to.titrate.acid.only; del&switch
108 .LT. (MINABU*1.d-6) moles B4O5(OH)4=               B4O5(OH)4=; del&switch
109 .LT. (MINABU*1.d-6) moles B3O3(OH)4-               B3O3(OH)4-; del&switch
110 pH (-log[aH+]); pmH(-log[mH+])      12.8532       12.7140
111 fCO2(g); log[fCO2(g)]=                                    6.983E-13    -12.2
112 Total Diagonal Inversions            84
113 Total Stoichiometric Reoptimizations             9
114 SINGLE BATCH EQUILIBRATION COMPLETED
```

Appendix B: Sample Screen Display of Np_NaCl_BM_LOG

See Table 4 for explanation of this screen display.

```
Enter chemdat file name to search on: np_am
Enter rhomin file name to search on: np_am
Enter input file name (without .extension): np_nacl_bm_log
%CMS-I-LIBIS, library is WP$NONPA_CMSROOT:[FMT]
%CMS-S-LIBSET, library set
-CMS-I-SUPERSEDE, library list superseded

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.CHEMDAT *Initial load*
FMT_HMW_NP_AM_960823.CHEMDAT *CHEMDAT DATABASE FILE FOR FMT 2.2 REGRESSION TESTING*
FMT_HMW_NP_AM_F60.CHEMDAT *Initial load*
FMT_HMW_NP_AM_RTEST.CHEMDAT *CHEMDAT DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING*
Select CHEMDAT name from list above: FMT_HMW_NP_AM_RTEST.CHEMDAT
Your CMS library list consists of:
    WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.RHOMIN *Initial load*
FMT_HMW_NP_AM_960823.RHOMIN *RHOMIN DATABASE FILE FOR FMT 2.2 REGRESSION TESTING*
FMT_HMW_NP_AM_RTEST.RHOMIN *RHOMIN DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING*
Select RHOMIN name from list above: FMT_HMW_NP_AM_RTEST.RHOMIN
Your CMS library list consists of:
    WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.RHOMIN fetched
Enter "Y" or "y" to echo database in OUT file: n

                image name: "FMT_PA97"
                image file identification: "P PA97 2.3"
                image file build identification: ""
                link date/time:  1-APR-1997 09:55:34.40
                linker identification: "A11-14"

DG_BYPASS flag set to nDG_BYPASS
Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

Accuracy of reactions is              1.0000E-06
Minimum elemental abundance is        1.0000E-18
Number of Aqueous Species is            50

ACTIVITY COEF. FLAG PITZACT
PITZER Data Base NOT Echoed in this Run
Finished do 10:  read b(0) b(1) b(2) cphi
Finished do 20:  read theta(c,c)
Finished do 30:  read theta(a,a)
Finished do 40:  read psi(c,c,a)
Finished do 50:  read psi(a,a,c)
Finished do 55:  read neucat(n,c)
Finished do 65:  read neuani(n,a)
Finished do 66:  read ptztsi(n,c,a)
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

Char Flags: FLOW/BATCH/TITRATE:  TITRATE    EXPLICIT
this is a TITRATION problem

Character Flags:  J.C. nMOLES     nEXACT
Character Flags:  I.C. nMOLES     nEXACT
pH (-log[aH+]); pmH(-log[mH+])      11.7497       11.6199
fCO2(g); log[fCO2(g)]=                                      2.171E-07    -6.66
pH (-log[aH+]); pmH(-log[mH+])       5.3205        5.9141
fCO2(g); log[fCO2(g)]=                                      3.400E-02    -1.47
TITRATION Character Flags
  cdum1= TITRATE      cdum2= LOG10
  First Volume Added =          0.10 mL
  Final Volume Added =         10.00 mL

pH (-log[aH+]); pmH(-log[mH+])       5.3205        5.9141
fCO2(g); log[fCO2(g)]=                                      3.400E-02    -1.47
pH (-log[aH+]); pmH(-log[mH+])       5.6451        6.2386
fCO2(g); log[fCO2(g)]=                                      2.716E-02    -1.57
pH (-log[aH+]); pmH(-log[mH+])       5.9936        6.5870
fCO2(g); log[fCO2(g)]=                                      1.847E-02    -1.73
pH (-log[aH+]); pmH(-log[mH+])       7.9427        8.5360
fCO2(g); log[fCO2(g)]=                                      3.555E-04    -3.45
pH (-log[aH+]); pmH(-log[mH+])       8.8722        9.4653
fCO2(g); log[fCO2(g)]=                                      4.250E-05    -4.37
```

Appendix B: Sample Screen Display of Np_NaCl_BM_LOG

```
84 pH (-log[aH+]); pmH(-log[mH+])      9.2225      9.8154
85 fCO2(g); log[fCO2(g)]=                                    1.922E-05    -4.72
86 pH (-log[aH+]); pmH(-log[mH+])      9.4695     10.0620
87 fCO2(g); log[fCO2(g)]=                                    1.108E-05    -4.96
88 pH (-log[aH+]); pmH(-log[mH+])      9.6719     10.2640
89 fCO2(g); log[fCO2(g)]=                                    7.112E-06    -5.15
90 pH (-log[aH+]); pmH(-log[mH+])      9.8493     10.4406
91 fCO2(g); log[fCO2(g)]=                                    4.873E-06    -5.31
92 pH (-log[aH+]); pmH(-log[mH+])     10.0098     10.6002
93 fCO2(g); log[fCO2(g)]=                                    3.501E-06    -5.46
94 pH (-log[aH+]); pmH(-log[mH+])     10.1578     10.7468
95 fCO2(g); log[fCO2(g)]=                                    2.614E-06    -5.58
96 pH (-log[aH+]); pmH(-log[mH+])     10.2955     10.8825
97 fCO2(g); log[fCO2(g)]=                                    2.019E-06    -5.69
98 pH (-log[aH+]); pmH(-log[mH+])     10.4243     11.0086
99 fCO2(g); log[fCO2(g)]=                                    1.608E-06    -5.79
100 pH (-log[aH+]); pmH(-log[mH+])    10.5454     11.1257
101 fCO2(g); log[fCO2(g)]=                                   1.317E-06    -5.88
102 pH (-log[aH+]); pmH(-log[mH+])    10.6594     11.2341
103 fCO2(g); log[fCO2(g)]=                                   1.106E-06    -5.96
104 End of AutoTitration Problem
```

Appendix C: Sample Screen Display of Np_NaCl_BM_LIN

Note

Lightened text same as screen display provided in Appendix B.

See Table 4 for explanation of this screen display.

```
1 Enter chemdat file name to search on: np_am
2 Enter rhomin file name to search on: np_am
3 Enter input file name (without .extension): np_nacl_bm_lin
4 %CMS-I-LIBIS, library is WP$NONPA_CMSROOT:[FMT]
5 %CMS-S-LIBSET, library set
6 -CMS-I-SUPERSEDE, library list superseded
7
8 Elements in CMS Library WP$NONPA_CMSROOT:[FMT]
9
10 FMT_HMW_NP_AM.CHEMDAT "Initial load"
11 FMT_HMW_NP_AM_960823.CHEMDAT "CHEMDAT DATABASE FILE FOR FMT 2.2 REGRESSION TESTING"
12 FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
13 FMT_HMW_NP_AM_RTEST.CHEMDAT "CHEMDAT DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING"
14 Select CHEMDAT name from list above: FMT_HMW_NP_AM_RTEST.CHEMDAT
15 Your CMS library list consists of:
16    WP$NONPA_CMSROOT:[FMT]
17
18 %CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched
19
20 Elements in CMS Library WP$NONPA_CMSROOT:[FMT]
21
22 FMT_HMW_NP_AM.RHOMIN "Initial load"
23 FMT_HMW_NP_AM_960823.RHOMIN "RHOMIN DATABASE FILE FOR FMT 2.2 REGRESSION TESTING"
24 FMT_HMW_NP_AM_RTEST.RHOMIN "RHOMIN DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING"
25 Select RHOMIN name from list above: FMT_HMW_NP_AM_RTEST.RHOMIN
26 Your CMS library list consists of:
27    WP$NONPA_CMSROOT:[FMT]
28
29 %CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.RHOMIN fetched
30 Enter "Y" or "y" to echo database in OUT file: n
31
32                image name: "FMT_PA97"
33                image file identification: "P PA97 2.3"
34                image file build identification: ""
35                link date/time:  1-APR-1997 09:55:34.40
36                linker identification: "A11-14"
37
38 DG_BYPASS flag set to nDG_BYPASS
39 Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
40 DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
41 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
42
43 Accuracy of reactions is              1.0000E-06
44 Minimum elemental abundance is       1.0000E-18
45 Number of Aqueous Species is           50
46
47 ACTIVITY COEF. FLAG PITZACT
48 PITZER Data Base NOT Echoed in this Run
49 Finished do 10:  read b(0) b(1) b(2) cphi
50 Finished do 20:  read theta(c,c)
51 Finished do 30:  read theta(a,a)
52 Finished do 40:  read psi(c,c,a)
53 Finished do 50:  read psi(a,a,c)
54 Finished do 55:  read neucat(n,c)
55 Finished do 65:  read neuani(n,a)
56 Finished do 66:  read ptztsi(n,c,a)
57 using PITZER ACTIVITY COEFFICIENT model
58 Charge Balance replaces element Oxygen
59
60 Char Flags: FLOW/BATCH/TITRATE:  TITRATE    EXPLICIT
61 this is a TITRATION problem
62
63 Character Flags:  J.C. nMOLES     nEXACT
64 Character Flags:  I.C. nMOLES     nEXACT
65 pH (-log[aH+]); pmH(-log[mH+])     11.7497       11.6199
66 fCO2(g); log[fCO2(g)]=                                    2.171E-07    -6.66
67 pH (-log[aH+]); pmH(-log[mH+])      5.3205        5.9141
68 fCO2(g); log[fCO2(g)]=                                    3.400E-02    -1.47
69 TITRATION Character Flags
70   cdum1= TITRATE       cdum2= LINEAR
71   First Volume Added =          0.10 mL
```

Appendix C Sample Screen Display of Np_NaCl_BM_LIN

```
 72   Final Volume Added =          1.40 mL
 73
 74 pH (-log[aH+]); pmH(-log[mH+])      5.3205      5.9141
 75 fCO2(g); log[fCO2(g)]=                                    3.400E-02    -1.47
 76 pH (-log[aH+]); pmH(-log[mH+])      5.6451      6.2386
 77 fCO2(g); log[fCO2(g)]=                                    2.716E-02    -1.57
 78 pH (-log[aH+]); pmH(-log[mH+])      7.8183      8.4116
 79 fCO2(g); log[fCO2(g)]=                                    4.720E-04    -3.33
 80 pH (-log[aH+]); pmH(-log[mH+])      8.9167      9.5098
 81 fCO2(g); log[fCO2(g)]=                                    3.841E-05    -4.42
 82 pH (-log[aH+]); pmH(-log[mH+])      9.1977      9.7906
 83 fCO2(g); log[fCO2(g)]=                                    2.033E-05    -4.69
 84 pH (-log[aH+]); pmH(-log[mH+])      9.3641      9.9569
 85 fCO2(g); log[fCO2(g)]=                                    1.400E-05    -4.85
 86 pH (-log[aH+]); pmH(-log[mH+])      9.4821     10.0747
 87 fCO2(g); log[fCO2(g)]=                                    1.077E-05    -4.97
 88 pH (-log[aH+]); pmH(-log[mH+])      9.5733     10.1656
 89 fCO2(g); log[fCO2(g)]=                                    8.815E-06    -5.05
 90 pH (-log[aH+]); pmH(-log[mH+])      9.6473     10.2395
 91 fCO2(g); log[fCO2(g)]=                                    7.501E-06    -5.12
 92 pH (-log[aH+]); pmH(-log[mH+])      9.7095     10.3015
 93 fCO2(g); log[fCO2(g)]=                                    6.558E-06    -5.18
 94 pH (-log[aH+]); pmH(-log[mH+])      9.7631     10.3548
 95 fCO2(g); log[fCO2(g)]=                                    5.848E-06    -5.23
 96 pH (-log[aH+]); pmH(-log[mH+])      9.8100     10.4016
 97 fCO2(g); log[fCO2(g)]=                                    5.293E-06    -5.28
 98 pH (-log[aH+]); pmH(-log[mH+])      9.8517     10.4431
 99 fCO2(g); log[fCO2(g)]=                                    4.848E-06    -5.31
100 pH (-log[aH+]); pmH(-log[mH+])      9.8892     10.4804
101 fCO2(g); log[fCO2(g)]=                                    4.483E-06    -5.35
102 pH (-log[aH+]); pmH(-log[mH+])      9.9232     10.5142
103 fCO2(g); log[fCO2(g)]=                                    4.178E-06    -5.38
104 End of AutoTitration Problem
```

Appendix D: Sample Screen Display of Np_NaCl_BM

Note

Lightened text same as screen display provided in Appendix B.

See Table 4 for explanation of this screen display.

```
1 Enter chemdat file name to search on: np_am
2 Enter rhomin file name to search on: np_am
3 Enter input file name (without .extension): np_nacl_bm
4 %CMS-I-LIBIS, library is WP$NONPA_CMSROOT:[FMT]
5 %CMS-S-LIBSET, library set
6 -CMS-I-SUPERSEDE, library list superseded
7
8 Elements in CMS Library WP$NONPA_CMSROOT:[FMT]
9
10 FMT_HMW_NP_AM.CHEMDAT "Initial load"
11 FMT_HMW_NP_AM_960823.CHEMDAT "CHEMDAT DATABASE FILE FOR FMT 2.2 REGRESSION TESTING"
12 FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
13 FMT_HMW_NP_AM_RTEST.CHEMDAT "CHEMDAT DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING"
14 Select CHEMDAT name from list above: FMT_HMW_NP_AM_RTEST.CHEMDAT
15 Your CMS library list consists of:
16    WP$NONPA_CMSROOT:[FMT]
17
18 %CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched
19
20 Elements in CMS Library WP$NONPA_CMSROOT:[FMT]
21
22 FMT_HMW_NP_AM.RHOMIN "Initial load"
23 FMT_HMW_NP_AM_960823.RHOMIN "RHOMIN DATABASE FILE FOR FMT 2.2 REGRESSION TESTING"
24 FMT_HMW_NP_AM_RTEST.RHOMIN "RHOMIN DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING"
25 Select RHOMIN name from list above: FMT_HMW_NP_AM_RTEST.RHOMIN
26 Your CMS library list consists of:
27    WP$NONPA_CMSROOT:[FMT]
28
29 %CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.RHOMIN fetched
30 Enter "Y" or "y" to echo database in OUT file: n
31
32                image name: "FMT_PA97"
33                image file identification: "P PA97 2.3"
34                image file build identification: ""
35                link date/time:  1-APR-1997 09:55:34.40
36                linker identification: "A11-14"
37
38 DG_BYPASS flag set to nDG_BYPASS
39 Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.6imolal NaCl                FMT V2.3
40 DATABASE:   HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
41 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
42
43 Accuracy of reactions is              1.0000E-06
44 Minimum elemental abundance is        1.0000E-18
45 Number of Aqueous Species is            50
46
47 ACTIVITY COEF. FLAG PITZACT
48 PITZER Data Base NOT Echoed in this Run
49 Finished do 10:  read b(0) b(1) b(2) cphi
50 Finished do 20:  read theta(c,c)
51 Finished do 30:  read theta(a,a)
52 Finished do 40:  read psi(c,c,a)
53 Finished do 50:  read psi(a,a,c)
54 Finished do 55:  read neucat(n,c)
55 Finished do 65:  read neuani(n,a)
56 Finished do 66:  read ptztsi(n,c,a)
57 using PITZER ACTIVITY COEFFICIENT model
58 Charge Balance replaces element Oxygen
59
60 Char Flags: FLOW/BATCH/TITRATE:  TITRATE    EXPLICIT
61 this is a TITRATION problem
62
63 Character Flags:  J.C. nMOLES     nEXACT
64 Character Flags:  I.C. nMOLES     nEXACT
65 pH (-log[aH+]); pmH(-log[mH+])     11.7497      11.6199
66 fCO2(g); log[fCO2(g)]=                                    2.171E-07    -6.66
67 pH (-log[aH+]); pmH(-log[mH+])      5.3205       5.9141
68 fCO2(g); log[fCO2(g)]=                                    3.400E-02    -1.47
69 TITRATION Character Flags
70   cdum1= TITRATE      cdum2= ASREAD
71 reading titrant volumes from input file
```

```
  First Volume Added =          0.10 mL
  Final Volume Added =         10.00 mL

pH (-log[aH+]); pmH(-log[mH+])      5.3205      5.9141
fCO2(g); log[fCO2(g)]=                                    3.400E-02    -1.47
pH (-log[aH+]); pmH(-log[mH+])      5.6451      6.2386
fCO2(g); log[fCO2(g)]=                                    2.716E-02    -1.57
pH (-log[aH+]); pmH(-log[mH+])      5.9936      6.5870
fCO2(g); log[fCO2(g)]=                                    1.847E-02    -1.73
pH (-log[aH+]); pmH(-log[mH+])      6.2353      6.8286
fCO2(g); log[fCO2(g)]=                                    1.290E-02    -1.89
pH (-log[aH+]); pmH(-log[mH+])      6.6996      7.2930
fCO2(g); log[fCO2(g)]=                                    5.484E-03    -2.26
pH (-log[aH+]); pmH(-log[mH+])      7.9427      8.5359
fCO2(g); log[fCO2(g)]=                                    3.555E-04    -3.45
pH (-log[aH+]); pmH(-log[mH+])      8.3317      8.9250
fCO2(g); log[fCO2(g)]=                                    1.461E-04    -3.84
pH (-log[aH+]); pmH(-log[mH+])      8.5655      9.1587
fCO2(g); log[fCO2(g)]=                                    8.559E-05    -4.07
pH (-log[aH+]); pmH(-log[mH+])      8.7166      9.3098
fCO2(g); log[fCO2(g)]=                                    6.060E-05    -4.22
pH (-log[aH+]); pmH(-log[mH+])      8.8722      9.4653
fCO2(g); log[fCO2(g)]=                                    4.250E-05    -4.37
pH (-log[aH+]); pmH(-log[mH+])      9.2225      9.8154
fCO2(g); log[fCO2(g)]=                                    1.922E-05    -4.72
pH (-log[aH+]); pmH(-log[mH+])      9.4695     10.0620
fCO2(g); log[fCO2(g)]=                                    1.108E-05    -4.96
pH (-log[aH+]); pmH(-log[mH+])      9.8493     10.4406
fCO2(g); log[fCO2(g)]=                                    4.873E-06    -5.31
pH (-log[aH+]); pmH(-log[mH+])     10.2955     10.8825
fCO2(g); log[fCO2(g)]=                                    2.019E-06    -5.69
pH (-log[aH+]); pmH(-log[mH+])     10.6594     11.2341
fCO2(g); log[fCO2(g)]=                                    1.106E-06    -5.96
End of AutoTitration Problem
```

Appendix E: Sample Input File "BATCH_DOC.IN"

See Table 5 for explanation of this listing.

```
1       '[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs'
2       'CHEMFILE'
3
4       'BATCH', 'UNUSED'
5
6       'nMOLES', 'nEXACT',
7         1.10222364E+02   Hydrogen
8         5.51654821E+01   Oxygen
9         2.00000000E-01   Sodium
10        1.00000000E-02   Potassium
11        1.00000000E-03   Magnesium
12        1.00000000E-04   Calcium
13        1.10000000E-01   Chlorine
14        1.00000000E-03   Sulfur
15        1.00000000E-04   Carbon
16        0.00000000E+00   PosIon
17        0.00000000E+00   NegIon
18        0.00000000E+00   Air
19        1.00000000E-07   Boron
20        0.00000000E+00   Bromine
21        0.00000000E+00   TracerEl
22        0.00000000E+00   Th(IV)
23        0.00000000E+00   Am(III)
24        0.00000000E+00   U(VI)
25        0.00000000E+00   Np(V)
26        0.00000000E+00   ClO4-(EL)
27        0.00000000E+00   Phosphorus
28        0.00000000E+00   Electron
29        4.90605392E-17   Charge
```

Appendix F: Sample Input File "Np_NaCl_BM_LOG.IN"

See Table 6 for explanation of this listing.

```
'Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl'
'CHEMFILE'

'TITRATE', 'EXPLICIT',

'nMOLES', 'nEXACT',
  1.11017363E+02   Hydrogen
  6.15086815E+01   Oxygen
  5.61000000E+00   Sodium
  0.00000000E+00   Potassium
  0.00000000E+00   Magnesium
  0.00000000E+00   Calcium
  1.61000000E+00   Chlorine
  0.00000000E+00   Sulfur
  2.00000001E+00   Carbon
  0.00000000E+00   PosIon
  0.00000000E+00   NegIon
  0.00000000E+00   Air
  0.00000000E+00   Boron
  0.00000000E+00   Bromine
  0.00000000E+00   TracerEl
  0.00000000E+00   Th(IV)
  0.00000000E+00   Am(III)
  0.00000000E+00   U(VI)
  0.00000000E+00   Np(V)
  0.00000000E+00   ClO4-(EL)
  0.00000000E+00   Phosphorus
  0.00000000E+00   Electron
 -2.22044605E-15   Charge

'nMOLES','nEXACT',
  1.11018363E+02   Hydrogen
  1.05508682E+02   Oxygen
  1.56100000E+01   Sodium
  0.00000000E+00   Potassium
  0.00000000E+00   Magnesium
  0.00000000E+00   Calcium
  5.61100000E+00   Chlorine
  0.00000000E+00   Sulfur
  1.00000000E+01   Carbon
  0.00000000E+00   PosIon
  0.00000000E+00   NegIon
  0.00000000E+00   Air
  0.00000000E+00   Boron
  0.00000000E+00   Bromine
  0.00000000E+00   TracerEl
  0.00000000E+00   Th(IV)
  0.00000000E+00   Am(III)
  0.00000000E+00   U(VI)
  1.00000000E+01   Np(V)
  0.00000000E+00   ClO4-(EL)
  0.00000000E+00   Phosphorus
  0.00000000E+00   Electron
 -2.37316632E-15   Charge

 15  2.25d3  0.0025d0  1.800001d5 'nDXVARIABLE'
'nDIFFUS',
'CONVEC',
```

Appendix F: Sample Input File "Np_NaCl_BM_LOG.IN"

```
'nSSDIFF',
'nRESTART',
'nPUSHPULL','nMULTINJ',

 20 1 20 'nLOTS' 10
'nTGRAD' 'LINEAR'
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'
 3
 0.1d0 0.2d0 0.3d0
 1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'
'nMOLES' 'nEXACT' Plain old pure H2O
  1.11017364E+02   Hydrogen
  5.55086820E+01   Oxygen
  0.00000000E+00   Sodium
  0.00000000E+00   Potassium
  0.00000000E+00   Magnesium
  0.00000000E+00   Calcium
  0.00000000E+00   Chlorine
  0.00000000E+00   Sulfur
  0.00000000E+00   Carbon
  0.00000000E+00   PosIon
  0.00000000E+00   NegIon
  0.00000000E+00   Air
  0.00000000E+00   Boron
  0.00000000E+00   Bromine
  0.00000000E+00   TracerEl
  0.00000000E+00   Pu(III)
  0.00000000E+00   Am(III)
  0.00000000E+00   U(VI)
  0.00000000E+00   Np(V)
  0.00000000E+00   ClO4-(EL)
  0.00000000E+00   Phosphorus
  0.00000000E+00   Electron
  0.00000000E+00   Charge

 1.d-12 1.d-20 (fracture, matrix permeabilities)
'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)
'VAR_AQ_RHO' 1074.9d0
'nNO X DIFF',
'UNIFORM',0

'TITRATE','LOG10',0.1d0,10.d0,'nINJSOLIDS'
```

Appendix G: Sample Input File "Np_NaCl_BM_LIN.IN"

Note

Lines 2 through 98 in this file (lightened text) same as lines 2 through 98 in file provided in Appendix F (NP_NaCl_BM_LOG.IN).

See Table 6 for explanation of this listing.

```
1 'Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl'
2 'CHEMFILE'
3
4 'TITRATE', 'EXPLICIT',
5
6  'nMOLES', 'nEXACT',
7    1.11017363E+02   Hydrogen
8    6.15086815E+01   Oxygen
9    5.61000000E+00   Sodium
10   0.00000000E+00   Potassium
11   0.00000000E+00   Magnesium
12   0.00000000E+00   Calcium
13   1.61000000E+00   Chlorine
14   0.00000000E+00   Sulfur
15   2.00000001E+00   Carbon
16   0.00000000E+00   PosIon
17   0.00000000E+00   NegIon
18   0.00000000E+00   Air
19   0.00000000E+00   Boron
20   0.00000000E+00   Bromine
21   0.00000000E+00   TracerEl
22   0.00000000E+00   Th(IV)
23   0.00000000E+00   Am(III)
24   0.00000000E+00   U(VI)
25   0.00000000E+00   Np(V)
26   0.00000000E+00   ClO4-(EL)
27   0.00000000E+00   Phosphorus
28   0.00000000E+00   Electron
29  -2.22044605E-15   Charge
30
31 'nMOLES','nEXACT',
32   1.11018363E+02   Hydrogen
33   1.05508682E+02   Oxygen
34   1.56100000E+01   Sodium
35   0.00000000E+00   Potassium
36   0.00000000E+00   Magnesium
37   0.00000000E+00   Calcium
38   5.61100000E+00   Chlorine
39   0.00000000E+00   Sulfur
40   1.00000000E+01   Carbon
41   0.00000000E+00   PosIon
42   0.00000000E+00   NegIon
43   0.00000000E+00   Air
44   0.00000000E+00   Boron
45   0.00000000E+00   Bromine
46   0.00000000E+00   TracerEl
47   0.00000000E+00   Th(IV)
48   0.00000000E+00   Am(III)
```

Appendix G: Sample Input File "NP_NaCl_BM_LIN.IN"

```
 0.00000000E+00   U(VI)
 1.00000000E+01   Np(V)
 0.00000000E+00   ClO4-(EL)
 0.00000000E+00   Phosphorus
 0.00000000E+00   Electron
-2.37316632E-15  Charge

 15  2.25d3  0.0025d0  1.800001d5 'nDXVARIABLE'
'nDIFFUS',
'CONVEC',
'nSSDIFF',
'nRESTART',
'nPUSHPULL','nMULTINJ',

 20 1 20 'nLOTS' 10
'nTGRAD' 'LINEAR'
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'
 3
 0.1d0 0.2d0 0.3d0
 1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'
'nMOLES' 'nEXACT' Plain old pure H2O
 1.11017364E+02   Hydrogen
 5.55086820E+01   Oxygen
 0.00000000E+00   Sodium
 0.00000000E+00   Potassium
 0.00000000E+00   Magnesium
 0.00000000E+00   Calcium
 0.00000000E+00   Chlorine
 0.00000000E+00   Sulfur
 0.00000000E+00   Carbon
 0.00000000E+00   PosIon
 0.00000000E+00   NegIon
 0.00000000E+00   Air
 0.00000000E+00   Boron
 0.00000000E+00   Bromine
 0.00000000E+00   TracerEl
 0.00000000E+00   Pu(III)
 0.00000000E+00   Am(III)
 0.00000000E+00   U(VI)
 0.00000000E+00   Np(V)
 0.00000000E+00   ClO4-(EL)
 0.00000000E+00   Phosphorus
 0.00000000E+00   Electron
 0.00000000E+00   Charge

 1.d-12 1.d-20 (fracture, matrix permeabilities)
'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)
'VAR_AQ_RHO' 1074.9d0
'nNO X DIFF',
'UNIFORM',0

'TITRATE','LINEAR',.1,10,'nINJSOLIDS'
```

Appendix H: Sample Input File "Np_NaCl_BM.IN"

Note

Lines 2 through 98 in this file (lightened text) same as lines 2 through 98 in file provided in Appendix F (NP_NaCl_BM_LOG.IN).

See Table 6 for explanation of this listing.

```
1 'Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl'
2 'CHEMFILE'
3
4 'TITRATE', 'EXPLICIT',
5
6  'nMOLES', 'nEXACT',
7     1.11017363E+02    Hydrogen
8     6.15086815E+01    Oxygen
9     5.61000000E+00    Sodium
10    0.00000000E+00    Potassium
11    0.00000000E+00    Magnesium
12    0.00000000E+00    Calcium
13    1.61000000E+00    Chlorine
14    0.00000000E+00    Sulfur
15    2.00000001E+00    Carbon
16    0.00000000E+00    PosIon
17    0.00000000E+00    NegIon
18    0.00000000E+00    Air
19    0.00000000E+00    Boron
20    0.00000000E+00    Bromine
21    0.00000000E+00    TracerEl
22    0.00000000E+00    Th(IV)
23    0.00000000E+00    Am(III)
24    0.00000000E+00    U(VI)
25    0.00000000E+00    Np(V)
26    0.00000000E+00    ClO4-(EL)
27    0.00000000E+00    Phosphorus
28    0.00000000E+00    Electron
29   -2.22044605E-15   Charge
30
31  'nMOLES','nEXACT',
32     1.11018363E+02    Hydrogen
33     1.05508682E+02    Oxygen
34     1.56100000E+01    Sodium
35     0.00000000E+00    Potassium
36     0.00000000E+00    Magnesium
37     0.00000000E+00    Calcium
38     5.61100000E+00    Chlorine
39     0.00000000E+00    Sulfur
40     1.00000000E+01    Carbon
41     0.00000000E+00    PosIon
42     0.00000000E+00    NegIon
43     0.00000000E+00    Air
44     0.00000000E+00    Boron
45     0.00000000E+00    Bromine
46     0.00000000E+00    TracerEl
47     0.00000000E+00    Th(IV)
48     0.00000000E+00    Am(III)
```

Appendix H: Sample Input File "Np_NaCl_BM.IN"

```
  0.00000000E+00   U(VI)
  1.00000000E+01   Np(V)
  0.00000000E+00   ClO4-(EL)
  0.00000000E+00   Phosphorus
  0.00000000E+00   Electron
 -2.37316632E-15  Charge

 15  2.25d3  0.0025d0  1.800001d5 'nDXVARIABLE'
'nDIFFUS',
'CONVEC',
'nSSDIFF',
'nRESTART',
'nPUSHPULL','nMULTINJ',

 20 1 20 'nLOTS' 10
'nTGRAD' 'LINEAR'
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'
 3
 0.1d0 0.2d0 0.3d0
 1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'
'nMOLES' 'nEXACT' Plain old pure H2O
  1.11017364E+02   Hydrogen
  5.55086820E+01   Oxygen
  0.00000000E+00   Sodium
  0.00000000E+00   Potassium
  0.00000000E+00   Magnesium
  0.00000000E+00   Calcium
  0.00000000E+00   Chlorine
  0.00000000E+00   Sulfur
  0.00000000E+00   Carbon
  0.00000000E+00   PosIon
  0.00000000E+00   NegIon
  0.00000000E+00   Air
  0.00000000E+00   Boron
  0.00000000E+00   Bromine
  0.00000000E+00   TracerEl
  0.00000000E+00   Pu(III)
  0.00000000E+00   Am(III)
  0.00000000E+00   U(VI)
  0.00000000E+00   Np(V)
  0.00000000E+00   ClO4-(EL)
  0.00000000E+00   Phosphorus
  0.00000000E+00   Electron
  0.00000000E+00   Charge

 1.d-12 1.d-20 (fracture, matrix permeabilities)
'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)
'VAR_AQ_RHO' 1074.9d0
'nNO X DIFF',
'UNIFORM',0

'TITRATE','ASREAD',0.1d0,10.d0,'nINJSOLIDS'
 0.10000
 0.14251
 0.16
 0.18
 0.20309
 0.22
 0.24
 0.26
 0.28943
 0.41246
 0.58780
```

Appendix H: Sample Input File "Np_NaCl_BM.IN"

```
112  1.1938
113  3.4551
114  10.000
```

Appendix I: Listing of HMW_NP_AM_RTEST.CHEMDAT and References Cited in Listing

I.1 Listing

See Table 10 for explanation of this listing.

```
'DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);'
'95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)'

23 115 'nNEM T' 'nACTCOEF' 'nECHO' 'nABCD'
200 1.d-6 1.d-18
'NONE' 298.15 1.d0 1.d0

'Hydrogen' 'Oxygen' 'Sodium' 'Potassium' 'Magnesium' 'Calcium' 'Chlorine' 'Sulfur' 'Carbon' 'PosIon'
  'NegIon' 'Air' 'Boron' 'Bromine' 'TracerEl' 'Th(IV)' 'Am(III)' 'U(VI)' 'Np(V)' 'ClO4-(EL)'
  'Phosphorus' 'Electron' 'Charge'
1.0079 15.9994 22.98977 39.0983 24.305 40.08 35.453 32.06 12.011 0.0 0.0
   28.84 10.81 79.904 0.0 232.0381 243.0 238.029 237.0482 99.4506 30.974 0.0 0.0

'H2O                          WATER' 2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -95.6635     HMW84
'Na+                             Na+' 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -105.651     HMW84
'K+                               K+' 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -113.957     HMW84
'Ca++                           Ca++' 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2   1 -223.10      HMW84
'Mg++                           Mg++' 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2   1 -183.468     HMW84
'MgOH+                         MgOH+' 1 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -251.94      HMW84
'H+                               H+' 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1  0.          HMW84

'Cl-                             Cl-' 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -52.955     HMW84
'SO4=                           SO4=' 0 4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2   1 -300.386    HMW84
'HSO4-                         HSO4-' 1 4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -304.942    HMW84
'OH-                             OH-' 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -63.435     HMW84
'HCO3-                         HCO3-' 1 3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -236.751    HMW84
'CO3=                           CO3=' 0 3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 -2   1 -212.944    HMW84

'CO2(aq)                     CO2(aq)' 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -155.68     HMW84
'CaCO3(aq)                 CaCO3(aq)' 0 3 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -443.5       HMW84
'MgCO3(aq)                 MgCO3(aq)' 0 3 0 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -403.155     HMW84

'B(OH)3(aq)               B(OH)3(aq)' 3 3 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0  0   1 -390.81      FW86
'B(OH)4-                   B(OH)4-' 4 4 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 -1   1 -465.20      FW86
'B3O3(OH)4-               B3O3(OH)4-' 4 7 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 -1   1 -963.77      FW86
'B4O5(OH)4=               B4O5(OH)4=' 4 9 0 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 -2   1 -1239.10     FW86
'CaB(OH)4+                 CaB(OH)4+' 4 4 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0  1   1 -692.30      FW86
'MgB(OH)4+                 MgB(OH)4+' 4 4 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0  1   1 -651.89      FW86
'Br-                             Br-' 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 -1   1 -999.99     arbitrary
'ClO4-                 perchlorate ClO4-' 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -1   1 -999.99     arbitrary

'NaOH(aq).....to.titrate.base.only' 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1  500.        arbitrary
'HCl(aq).....to.titrate.acid.only' 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1  500.        arbitrary
'HClO4(aq).....to.titrate.acid.only' 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0  0   1  500.        arbitrary
'PosIon.................POSITIVE.ION' 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0  1   1  0.          arbitrary
'NegIon.................NEGATIVE.ION' 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 -1   1  0.          arbitrary
'PosIon(OH)(aq).....to.titrate.base' 1 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0  0   1  500.        arbitrary
'HNegIon(aq).....to.titrate.acid' 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  0   1  500.        arbitrary
'Tracer(aq).....conservative.tracer' 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0  0   1  0.          arbitrary

'H3PO4(aq)                 H3PO4(aq)' 3 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0  0   1 -460.90      RFF92
'H2PO4-                     H2PO4-' 2 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -1   1 -455.96      RFF92
'HPO4=                       HPO4=' 1 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -2   1 -439.367     RFF94
'PO4=-                       PO4=-' 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -3   1 -410.947     RFF94

'NpO2+                       NpO2+' 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0  1   1 -369.127     N&R94
'NpO2OH(aq)               NpO2OH(aq)' 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0  0   1 -438.518     N&R94
'NpO2(OH)2-               NpO2(OH)2-' 2 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 -1   1 -505.829     N&R94
'NpO2CO3-                 NpO2CO3-' 0 5 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 -1   1 -594.492     N&R94
'NpO2(CO3)2=-           NpO2(CO3)2=-' 0 8 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 1 0 0 0 -3   1 -808.403     N&R94
'NpO2(CO3)3=5-         NpO2(CO3)3=5-' 0 11 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 -5  1 -1019.918    N&R94

'Am+++                       Am+++' 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  3   1 -241.694     FRP90
'AmCO3+                     AmCO3+' 0 3 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0  1   1 -472.060     FRP90
'Am(CO3)2-                 Am(CO3)2-' 0 6 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 -1   1 -695.880     FRP90
'Am(CO3)3=-               Am(CO3)3=-' 0 9 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 1 0 0 0 0 0 -3   1 -915.460     FRP90
'Am(OH)2+                 Am(OH)2+' 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  1   1 -393.647     RFFR92
'Am(OH)3(aq)             Am(OH)3(aq)' 3 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  0   1 -462.950     RFFR92

'Th++++                     Th++++' 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0  4   1 -999.99      arbitrary

'UO2++                   U(VI)O2++' 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  2   1 -999.99      arbitrary

'NpO2OH(aged)_____NpO2OH(aged)' 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  0   2 -454.010     N&R94
'NpO2OH(amor)_____NpO2OH(amor)' 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  0   2 -452.642     N&R94
'NaNpO2CO3(s)_____NaNpO2CO3(s)' 0 5 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  0   2 -713.707     N&R94
'Na3NpO2(CO3)2(s)_DISABLED_DISABLED' 0 8 3 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  0   2  999.99     arbitrary

'AmOHCO3(c)_____AmOHCO3(c)' 1 4 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0  0   2 -569.980     FRP90
'Am(OH)3(s)_____Am(OH)3(s)' 3 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  0   2 -492.294     FRSR89
'NaAm(CO3)2.6H2O(c)_____' 12 12 1 0 0 0 0 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0  0   2 -1396.494    RRFF94
'AmPO4(c)_____AmPO4(c)' 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0  0   2 -709.750     RFF94

'CaSO4_____Anhydrite' 0 4 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -533.73      HMW84
'NaK3(SO4)2__Aphthitalite/Glaserite' 0 8 1 3 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1057.05    HMW84
'CaCl2.6H2O_____Antarcticite' 12 6 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -893.65     HMW84
'CaCO3_____Aragonite' 0 3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -455.17     HMW84
'K2SO4_____Arcanite' 0 4 0 2 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -532.39     HMW84
'MgCl2.6H2O_____Bischofite' 12 6 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -853.1      HMW84
'Na2Mg(SO4)2.4H2O_____Bloedite' 8 12 2 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1383.6     HMW84
'Mg(OH)2_____Brucite' 2 2 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -335.4      HMW84
'Na6CO3(SO4)2_____Burkeite' 0 11 6 0 0 0 0 2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1449.4     HMW84
'CaCO3_____Calcite' 0 3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -455.6      HMW84
'CaCl2.4H2O_____CaCl2_Tetrahydrite' 8 4 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -698.7      HMW84
'Ca4Cl2(OH)6.13H2O__CaOxychloride A' 32 19 0 0 0 4 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -2658.45    HMW84
'Ca2Cl2(OH)2.H2O____CaOxychloride B' 4 3 0 0 0 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -778.41     HMW84
'KMgCl3.6H2O_____Carnallite' 12 6 0 1 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1020.3     HMW84
'MgSO4.7H2O_____Epsomite' 14 11 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1157.83    HMW84
'CaNa2(CO3)2.5H2O_____Gaylussite' 10 11 2 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1360.5     HMW84
'Na2Ca(SO4)2_____Glauberite' 0 8 2 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1047.45    HMW84
'CaSO4.2H2O_____Gypsum' 4 6 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -725.56     HMW84
'NaCl_____Halite' 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -154.99     HMW84
'MgSO4.6H2O_____Hexahydrite' 12 10 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1061.60    HMW84
'KMgClSO4.3H2O_____Kainite' 6 7 0 1 1 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -938.2      HMW84
'KHCO3_____Kalicinite' 1 3 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -350.06     HMW84
```

Appendix I: Listing of HMW_NP_AM_RTEST.CHEMDAT and References Cited in Listing

```
'MgSO4.H2O_____Kieserite'  2  5 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -579.80     HMW84
'K2Mg(SO4)2.4H2O_____Leonite'  8 12 0 2 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1403.97   HMW84
'Na4Ca(SO4)3.2H2O_____Labile_Salt'  4 14 4 0 0 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1751.45   HMW84
'MgCO3_____Magnesite'  0  3 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -414.45    HMW84
'Mg2Cl(OH)3.4H2O_____MgOxychloride'  11  7 0 0 2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1029.6   HMW84
'KHSO4_____Mercallite'  1  4 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -417.57    HMW84
'Na2SO4.10H2O_____Mirabilite'  20 14 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1471.15   HMW84
'K8H5(SO4)7_____Misenite'  6 28 0 8 0 0 0 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -3039.24   HMW84
'NaHCO3_____Nahcolite'  1  3 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -343.33    HMW84
'Na2CO3.10H2O_____Natron'  20 13 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1282.78   HMW84
'MgCO3.3H2O_____Nesquehonite'  6  6 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -695.3    HMW84
'K2Mg(SO4)2.6H2O Picromerite/Schoen'  12 14 0 2 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1596.1   HMW84
'Na2Ca(CO3)2.2H2O_____Pirssonite'  4  8 2 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1073.1   HMW84
'K2MgCa2(SO4)4.2H2O_____Polyhalite'  4 18 0 2 1 2 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -2282.5   HMW84
'Ca(OH)2_____Portlandite'  2  2 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -362.12    HMW84
'K2CO3.3/2H2O___Potassium_Carbonate'  3 4.5 0 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -577.37   HMW84
'K8H4(CO3)6.3H2O___K-Sequicarbonate'  10 21 0 8 0 0 0 0 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -2555.4   HMW84
'KNaCO3.6H2O_____K-Na-Carbonate'  12  9 1 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1006.8   HMW84
'K2NaH(CO3)2.2H2O___Potassium_Trona'  5  8 1 2 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -971.74   HMW84
'K3H(SO4)2__Sesquipotassium_Sulfate'  1  8 0 3 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -950.8    HMW84
'Na3H(SO4)2____Sesquisodium_Sulfate'  1  8 3 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -919.6    HMW84
'Na2CO3.7H2O____Na2CO3-Heptahydrate'  14 10 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1094.95   HMW84
'KCl_____Sylvite'  0  0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -164.84    HMW84
'K2Ca(SO4)2.H2O_____Syngenite'  2  9 0 2 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1164.8   HMW84
'Mg2CaCl6.12H2O_____Tachyhydrite'  24 12 0 0 2 1 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -2015.9   HMW84
'Na2SO4_____Thenardite'  0  4 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -512.35   HMW84
'Na2CO3.H2O_____Thermonatrite'  2  4 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -518.6    HMW84
'Na3H(CO3)2.2H2O_____Trona'  5  8 3 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -960.38   HMW84
'Na2B4O7.10H2O_____Borax'  20 17 2 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0  2 -2224.16   PW86
'B(OH)3_____Borix_Acid_Solid'  3  3 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0  2 -390.86    PW86
'KB5O8.4H2O___K-Pentaborate_(30_C)'  8 12 0 1 0 0 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0  2 -1770.26   PW86
'K2B4O7.4H2O___K-Tetraborate_(30_C)'  8 11 0 2 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0  2 -1663.47   PW86
'NaBO2.4H2O_____Sodium_Metaborate'  8  6 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  2 -761.42    PW86
'NaB5O8.5H2O_____Sodium_Pentaborate'  10 13 1 0 0 0 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0  2 -1854.80   PW86
'NaBO2.NaCl.2H2O___Teepleite_(20_C)'  4  4 2 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  2 -725.77    PW86

'nDG_BYPASS' 0
'PITZACT'
 13 #Cat  Na,K,Ca,Mg,MgOH,H,MgB(OH)4+,CaB(OH)4+,Am+++,AmCO3+,Th++++,UO2++,NpO2+
 20 #Ani  Cl,SO4,HSO4,OH,HCO3,CO3,B(OH)4,B3O3(OH)4,B4O5(OH)4,Br,Am(CO3)2-,Am(CO3)3=-,ClO4-,NpO2(OH)2-,NpC,NpC2,NpC3,H2PO4,HPO4.PO4
  6 #Neu  CO2,CaCO3,MgCO3,B(OH)3,H3PO4

  1  .0765     .2644     .0      .00127    Na+ Cl-            HMW84 (beta0, beta1, beta2, cphi)
  1  .01958   1.113      .0      .00497    Na+ SO4=           HMW84
  1  .0454     .398      .0      .0        Na+ HSO4-          HMW84
  1  .0864     .253      .0      .0044     Na+ OH-            HMW84
  1  .0277     .0411     .0      .0        Na+ HCO3-          HMW84
  1  .0399    1.389      .0      .0044     Na+ CO3=           HMW84
  1 -.0427     .089      .0      .0114     Na+ B(OH)4-        PW86
  1 -.056     -.910      .0      .0        Na+ B3O3(OH)4-     PW86
  1 -.11      -.40       .0      .0        Na+ B4O5(OH)4=     PW86
  1  .0        .0        .0      .0        Na+ Br-
  1  .0      -8.37       .0      .0        Na+ Am(CO3)2-      RRFP94
  1 -.94      8.1        .0      .418      Na+ Am(CO3)3=-     RRFP94,PRP90
  1  .0554     .2755     .0     -.00118    Na+ ClO4-          P91
  1  .0        .0        .0      .0        Na+ NpO2(OH)2-     NR94
  1  .161      .0        .0      .0        Na+ NpO2CO3-       NR94
  1  .407      .0        .0      .0        Na+ NpO2(CO3)2=-   NR94
  1 1.97      16.        .0      .0        Na+ NpO2(CO3)3=-   NR94
  1 +.0533     .0396     .0      .00795    Na+ H2PO4-         P91
  1 -.0583    1.466      .0      .0294     Na+ HPO4=          P91
  1  .1781    3.851      .0     -.05154    Na+ PO4=-          P91

  1  .04835    .2122     .0     -.00084    K+ Cl-             HMW84
  1  .04995    .7793     .0      .0        K+ SO4=            HMW84
  1 -.0003     .1735     .0      .0        K+ HSO4-           HMW84
  1  .1298     .320      .0      .0041     K+ OH-             HMW84
  1  .0296    -.013      .0     -.008      K+ HCO3-           HMW84
  1  .1488    1.43       .0     -.0015     K+ CO3=            HMW84
  1  .035      .14       .0      .0        K+ B(OH)4-         PW86
  1 -.13       .0        .0      .0        K+ B3O3(OH)4-      PW86
  1 -.022      .0        .0      .0        K+ B4O5(OH)4=      PW86
  1  .0        .0        .0      .0        K+ Br-
  1  .0        .0        .0      .0        K+ Am(CO3)2-
  1  .0        .0        .0      .0        K+ Am(CO3)3=-
  1  .0        .0        .0      .0        K+ ClO4-
  1  .0        .0        .0      .0        K+ NpO2(OH)2-
  1  .0        .0        .0      .0        K+ NpO2CO3-
  1  .0        .0        .0      .0        K+ NpO2(CO3)2=-
  1  .0        .0        .0      .0        K+ NpO2(CO3)3=-=-
  1 -.0678    -.1042     .0      .0        K+ H2PO4-          P91
  1  .0248    1.274      .0      .0164     K+ HPO4=           P91
  1  .3729    3.972      .0     -.08680    K+ PO4=-           P91

  1  .3159    1.614      .0     -.00034    Ca++ Cl-           HMW84
  2  .20      3.1973   -54.24    .0        Ca++ SO4=          HMW84
  1  .2145    2.53       .0      .0        Ca++ HSO4-         HMW84
  1 -.1747    -.2303    -5.72    .0        Ca++ OH-           HMW84
  1  .4       2.977      .0      .0        Ca++ HCO3-         HMW84
  2  .0        .0        .0      .0        Ca++ CO3=          HMW84
  1  .0        .0        .0      .0        Ca++ B(OH)4-       PW86
  1  .0        .0        .0      .0        Ca++ B3O3(OH)4-    PW86
  1  .0        .0        .0      .0        Ca++ B4O5(OH)4=    PW86
  1  .0        .0        .0      .0        Ca++ Br-
  1  .0        .0        .0      .0        Ca++ Am(CO3)2-
  3  .0        .0        .0      .0        Ca++ Am(CO3)3=-
  1  .4511    1.756      .0     -.00500    Ca++ ClO4-         P91
  1  .0        .0        .0      .0        Ca++ NpO2(OH)2-
  1  .0        .0        .0      .0        Ca++ NpO2CO3-
  3  .0        .0        .0      .0        Ca++ NpO2(CO3)2=-
  3  .0        .0        .0      .0        Ca++ NpO2(CO3)3=-=-
  1  .0        .0        .0      .0        Ca++ H2PO4-
  2  .0        .0        .0      .0        Ca++ HPO4=
  3  .0        .0        .0      .0        Ca++ PO4=-

  1  .35235   1.6815     .0      .00519    Mg++ Cl-           HMW84
  2  .2210    3.343    -37.23    .025      Mg++ SO4=          HMW84
  1  .4746    1.729      .0      .0        Mg++ HSO4-         HMW84
  1  .0        .0        .0      .0        Mg++ OH-           HMW84
  1  .329      .6072     .0      .0        Mg++ HCO3-         HMW84
  2  .0        .0        .0      .0        Mg++ CO3=          HMW84
  1  .0        .0        .0      .0        Mg++ B(OH)4-       PW86
  1  .0        .0        .0      .0        Mg++ B3O3(OH)4-    PW86
  1  .0        .0        .0      .0        Mg++ B4O5(OH)4=    PW86
  1  .0        .0        .0      .0        Mg++ Br-
  1  .0        .0        .0      .0        Mg++ Am(CO3)2-
  3  .0        .0        .0      .0        Mg++ Am(CO3)3=-
  1  .4961    2.008      .0      .009578   Mg++ ClO4-         P91
  1  .0        .0        .0      .0        Mg++ NpO2(OH)2-
  1  .0        .0        .0      .0        Mg++ NpO2CO3-
  3  .0        .0        .0      .0        Mg++ NpO2(CO3)2=-
  3  .0        .0        .0      .0        Mg++ NpO2(CO3)3=-=-
  1  .0        .0        .0      .0        Mg++ H2PO4-
  2  .0        .0        .0      .0        Mg++ HPO4=
```

Appendix I: Listing of HMW_NP_AM_RTEST.CHEMDAT and References Cited in Listing

```
230     3  .0        .0        .0      .0       Mg++ PO4=-
231
232     1 -.10       1.658     .0      .0       MgOH+ Cl-              HMW84
233     1  .0        .0        .0      .0       MgOH+ SO4=             HMW84
234     1  .0        .0        .0      .0       MgOH+ HSO4-            HMW84
235     1  .0        .0        .0      .0       MgOH+ OH-              HMW84
236     1  .0        .0        .0      .0       MgOH+ HCO3-            HMW84
237     1  .0        .0        .0      .0       MgOH+ CO3=             HMW84
238     1  .0        .0        .0      .0       MgOH+ B(OH)4-
239     1  .0        .0        .0      .0       MgOH+ B3O3(OH)4-
240     1  .0        .0        .0      .0       MgOH+ B4O5(OH)4=
241     1  .0        .0        .0      .0       MgOH+ Br-
242     1  .0        .0        .0      .0       MgOH+ Am(CO3)2-
243     1  .0        .0        .0      .0       MgOH+ Am(CO3)3=-
244     1  .0        .0        .0      .0       MgOH+ ClO4-
245     1  .0        .0        .0      .0       MgOH+ NpO2(OH)2-
246     1  .0        .0        .0      .0       MgOH+ NpO2CO3-
247     1  .0        .0        .0      .0       MgOH+ NpO2(CO3)2=-
248     1  .0        .0        .0      .0       MgOH+ NpO2(CO3)3==-
249     1  .0        .0        .0      .0       MgOH+ H2PO4-
250     1  .0        .0        .0      .0       MgOH+ HPO4=
251     1  .0        .0        .0      .0       MgOH+ PO4=-
252
253     1  .1775     .2945     .0      .0008    H+ Cl-                 HMW84
254     1  .0298     .0        .0      .0438    H+ SO4=                HMW84
255     1  .2065     .5556     .0      .0       H+ HSO4-               HMW84
256     1  .0        .0        .0      .0       H+ OH-                 HMW84
257     1  .0        .0        .0      .0       H+ HCO3-               HMW84
258     1  .0        .0        .0      .0       H+ CO3=                HMW84
259     1  .0        .0        .0      .0       H+ B(OH)4-             FW86
260     1  .0        .0        .0      .0       H+ B3O3(OH)4-          FW86
261     1  .0        .0        .0      .0       H+ B4O5(OH)4=          FW86
262     1  .0        .0        .0      .0       H+ Br-
263     1  .0        .0        .0      .0       H+ Am(CO3)2-
264     1  .0        .0        .0      .0       H+ Am(CO3)3=-
265     1  .1747     .2931     .0      .00819   H+ ClO4-               P91
266     1  .0        .0        .0      .0       H+ NpO2(OH)2-
267     1  .0        .0        .0      .0       H+ NpO2CO3-
268     1  .0        .0        .0      .0       H+ NpO2(CO3)2=-
269     1  .0        .0        .0      .0       H+ NpO2(CO3)3==-
270     1  .0        .0        .0      .0       H+ H2PO4-
271     1  .0        .0        .0      .0       H+ HPO4=
272     1  .0        .0        .0      .0       H+ PO4=-
273
274     1  .16       .0        .0      .0       MgB(OH)4+ Cl-          HMW84
275     1  .0        .0        .0      .0       MgB(OH)4+ SO4=         HMW84
276     1  .0        .0        .0      .0       MgB(OH)4+ HSO4-        HMW84
277     1  .0        .0        .0      .0       MgB(OH)4+ OH-          HMW84
278     1  .0        .0        .0      .0       MgB(OH)4+ HCO3-        HMW84
279     1  .0        .0        .0      .0       MgB(OH)4+ CO3=         HMW84
280     1  .0        .0        .0      .0       MgB(OH)4+ B(OH)4-
281     1  .0        .0        .0      .0       MgB(OH)4+ B3O3(OH)4-
282     1  .0        .0        .0      .0       MgB(OH)4+ B4O5(OH)4=
283     1  .0        .0        .0      .0       MgB(OH)4+ Br-
284     1  .0        .0        .0      .0       MgB(OH)4+ Am(CO3)2-
285     1  .0        .0        .0      .0       MgB(OH)4+ Am(CO3)3=-
286     1  .0        .0        .0      .0       MgB(OH)4+ ClO4-
287     1  .0        .0        .0      .0       MgB(OH)4+ NpO2(OH)2-
288     1  .0        .0        .0      .0       MgB(OH)4+ NpO2CO3-
289     1  .0        .0        .0      .0       MgB(OH)4+ NpO2(CO3)2=-
290     1  .0        .0        .0      .0       MgB(OH)4+ NpO2(CO3)3==-
291     1  .0        .0        .0      .0       MgB(OH)4+ H2PO4-
292     1  .0        .0        .0      .0       MgB(OH)4+ HPO4=
293     1  .0        .0        .0      .0       MgB(OH)4+ PO4=-
294
295     1  .12       .0        .0      .0       CaB(OH)4+ Cl-
296     1  .0        .0        .0      .0       CaB(OH)4+ SO4=         HMW84
297     1  .0        .0        .0      .0       CaB(OH)4+ HSO4-        HMW84
298     1  .0        .0        .0      .0       CaB(OH)4+ OH-          HMW84
299     1  .0        .0        .0      .0       CaB(OH)4+ HCO3-        HMW84
300     1  .0        .0        .0      .0       CaB(OH)4+ CO3=         HMW84
301     1  .0        .0        .0      .0       CaB(OH)4+ B(OH)4-
302     1  .0        .0        .0      .0       CaB(OH)4+ B3O3(OH)4-
303     1  .0        .0        .0      .0       CaB(OH)4+ B4O5(OH)4=
304     1  .0        .0        .0      .0       CaB(OH)4+ Br-
305     1  .0        .0        .0      .0       CaB(OH)4+ Am(CO3)2-
306     1  .0        .0        .0      .0       CaB(OH)4+ Am(CO3)3=-
307     1  .0        .0        .0      .0       CaB(OH)4+ ClO4-
308     1  .0        .0        .0      .0       CaB(OH)4+ NpO2(OH)2-
309     1  .0        .0        .0      .0       CaB(OH)4+ NpO2CO3-
310     1  .0        .0        .0      .0       CaB(OH)4+ NpO2(CO3)2=-
311     1  .0        .0        .0      .0       CaB(OH)4+ NpO2(CO3)3==-
312     1  .0        .0        .0      .0       CaB(OH)4+ H2PO4-
313     1  .0        .0        .0      .0       CaB(OH)4+ HPO4=
314     1  .0        .0        .0      .0       CaB(OH)4+ PO4=-
315
316     1  .6117     5.403     .0     -0.0284   Am+++ Cl-              FRSR89
317     3 3.0398     .0      -2500     .0       Am+++ SO4=             RFF94
318     1  .0        .0        .0      .0       Am+++ HSO4-
319     1  .0        .0        .0      .0       Am+++ OH-
320     1  .0        .0        .0      .0       Am+++ HCO3-
321     3  .0        .0        .0      .0       Am+++ CO3=
322     1  .0        .0        .0      .0       Am+++ B(OH)4-
323     1  .0        .0        .0      .0       Am+++ B3O3(OH)4-
324     1  .0        .0        .0      .0       Am+++ B4O5(OH)4=
325     1  .0        .0        .0      .0       Am+++ Br-
326     1  .0        .0        .0      .0       Am+++ Am(CO3)2-
327     3  .0        .0        .0      .0       Am+++ Am(CO3)3=-
328     1  .80       5.35      .0     -0.0048   Am+++ ClO4-            FRF90
329     1  .0        .0        .0      .0       Am+++ NpO2(OH)2-
330     1  .0        .0        .0      .0       Am+++ NpO2CO3-
331     3  .0        .0        .0      .0       Am+++ NpO2(CO3)2=-
332     3  .0        .0        .0      .0       Am+++ NpO2(CO3)3==-
333     1  .0        .0      -92.9     .0       Am+++ H2PO4-           RFF94
334     3  .0        .0        .0      .0       Am+++ HPO4=
335     3  .0        .0        .0      .0       Am+++ PO4=-
336
337     1  .0        .0        .0      .0       AmCO3+ Cl-
338     1  .0        .0        .0      .0       AmCO3+ SO4=
339     1  .0        .0        .0      .0       AmCO3+ HSO4-
340     1  .0        .0        .0      .0       AmCO3+ OH-
341     1  .0        .0        .0      .0       AmCO3+ HCO3-
342     1  .0        .0        .0      .0       AmCO3+ CO3=
343     1  .0        .0        .0      .0       AmCO3+ B(OH)4-
344     1  .0        .0        .0      .0       AmCO3+ B3O3(OH)4-
345     1  .0        .0        .0      .0       AmCO3+ B4O5(OH)4=
346     1  .0        .0        .0      .0       AmCO3+ Br-
347     1  .0        .0        .0      .0       AmCO3+ Am(CO3)2-
348     1  .0        .0        .0      .0       AmCO3+ Am(CO3)3=-
349     1  .0        .0        .0      .0       AmCO3+ ClO4-
350     1  .0        .0        .0      .0       AmCO3+ NpO2(OH)2-
351     1  .0        .0        .0      .0       AmCO3+ NpO2CO3-
352     1  .0        .0        .0      .0       AmCO3+ NpO2(CO3)2=-
353     1  .0        .0        .0      .0       AmCO3+ NpO2(CO3)3==-
```

Appendix I: Listing of HMW_NP_AM_RTEST.CHEMDAT and References Cited in Listing

```
 1  .0       .0       .0     .0       AmCO3+ H2PO4-
 1  .0       .0       .0     .0       AmCO3+ HPO4=
 1  .0       .0       .0     .0       AmCO3+ PO4=-

 1  .0       .0       .0     .0       Th++++ Cl-
 3  .0       .0       .0     .0       Th++++ SO4=
 1  .0       .0       .0     .0       Th++++ HSO4-
 1  .0       .0       .0     .0       Th++++ OH-
 1  .0       .0       .0     .0       Th++++ HCO3-
 3  .0       .0       .0     .0       Th++++ CO3=
 1  .0       .0       .0     .0       Th++++ B(OH)4-
 1  .0       .0       .0     .0       Th++++ B3O3(OH)4-
 1  .0       .0       .0     .0       Th++++ B4O5(OH)4=
 1  .0       .0       .0     .0       Th++++ Br-
 1  .0       .0       .0     .0       Th++++ Am(CO3)2-
 3  .0       .0       .0     .0       Th++++ Am(CO3)3=-
 1  .0       .0       .0     .0       Th++++ ClO4-
 1  .0       .0       .0     .0       Th++++ NpO2(OH)2-
 1  .0       .0       .0     .0       Th++++ NpO2CO3-
 3  .0       .0       .0     .0       Th++++ NpO2(CO3)2=-
 3  .0       .0       .0     .0       Th++++ NpO2(CO3)3=5-
 1  .0       .0       .0     .0       Th++++ H2PO4-
 3  .0       .0       .0     .0       Th++++ HPO4=
 3  .0       .0       .0     .0       Th++++ PO4=-

 1  .4274    1.644    .0     -.03686  UO2++ Cl-            P91
 2  .322     1.827    .0     -.0176   UO2++ SO4=           P91
 1  .0       .0       .0     .0       UO2++ HSO4-
 1  .0       .0       .0     .0       UO2++ OH-
 1  .0       .0       .0     .0       UO2++ HCO3-
 2  .0       .0       .0     .0       UO2++ CO3=
 1  .0       .0       .0     .0       UO2++ B(OH)4-
 1  .0       .0       .0     .0       UO2++ B3O3(OH)4-
 1  .0       .0       .0     .0       UO2++ B4O5(OH)4=
 1  .0       .0       .0     .0       UO2++ Br-
 1  .0       .0       .0     .0       UO2++ Am(CO3)2-
 3  .0       .0       .0     .0       UO2++ Am(CO3)3=-
 1  .6113    2.144    .0     .02168   UO2++ ClO4-          P91
 1  .0       .0       .0     .0       UO2++ NpO2(OH)2-
 1  .0       .0       .0     .0       UO2++ NpO2CO3-
 3  .0       .0       .0     .0       UO2++ NpO2(CO3)2=-
 3  .0       .0       .0     .0       UO2++ NpO2(CO3)3=5-
 1  .0       .0       .0     .0       UO2++ H2PO4-
 2  .0       .0       .0     .0       UO2++ HPO4=
 3  .0       .0       .0     .0       UO2++ PO4=-

 1  0.169    .0       .0     .0       NpO2+ Cl-            NR94
 1  .0       .0       .0     .0       NpO2+ SO4=
 1  .0       .0       .0     .0       NpO2+ HSO4-
 1  .0       .0       .0     .0       NpO2+ OH-
 1  .0       .0       .0     .0       NpO2+ HCO3-
 1  .0       .0       .0     .0       NpO2+ CO3=
 1  .0       .0       .0     .0       NpO2+ B(OH)4-
 1  .0       .0       .0     .0       NpO2+ B3O3(OH)4-
 1  .0       .0       .0     .0       NpO2+ B4O5(OH)4=
 1  .0       .0       .0     .0       NpO2+ Br-
 1  .0       .0       .0     .0       NpO2+ Am(CO3)2-
 1  .0       .0       .0     .0       NpO2+ Am(CO3)3=-
 1  0.312    .0       .0     .0       NpO2+ ClO4-          NR94
 1  .0       .0       .0     .0       NpO2+ NpO2(OH)2-
 1  .0       .0       .0     .0       NpO2+ NpO2CO3-
 1  .0       .0       .0     .0       NpO2+ NpO2(CO3)2=-
 1  .0       .0       .0     .0       NpO2+ NpO2(CO3)3=5-
 1  .0       .0       .0     .0       NpO2+ H2PO4-
 1  .0       .0       .0     .0       NpO2+ HPO4=
 1  .0       .0       .0     .0       NpO2+ PO4=-


-.012 .07  .07   0.   .036 0.   0.  0.  0.  0.  0.  0.   Na:       (cations  2 thru 13)
 .032 0.   0.   .005 0.   0.   0.  0.  0.  0.  0.        K:       (cations  3 thru 13)
 .007 0.   .092 0.   0.   0.   0.  0.  0.  0.            Ca:      (cations  4 thru 13)
   0. .10  0.   0.   0.   0.   0.  0.  0.                Mg:      (cations  5 thru 13)
   0.  0.  0.   0.   0.   0.   0.  0.                    MgOH:    (cations  6 thru 13)
   0.  0.  0.   0.   0.   0.   0.                        H :      (cations  7 thru 13)
   0.  0.  0.   0.   0.   0.                             MgB(OH)4:(cations  8 thru 13)
   0.  0.  0.   0.   0.                                  CaB(OH)4:(cations  9 thru 13)
   0.  0.  0.   0.                                       Am+++:   (cations 10 thru 13)
   0.  0.  0.                                            AmCO3+:  (cations 11 thru 13)
   0.  0.                                                Th++++:  (cations 12 thru 13)
   0.                                                    UO2++:   (cations 13 thru 13)


 .02  -.006  -.050  .03  -.02  -.065 .12 .074 0. 0. 0. 0. 0. 0. 0. 0. .1  0. 0. Cl:          (anions  2-20)
 0.   -.013  .01   .02  -.012  .10  .12  0.  0. 0. 0. 0. 0. 0. 0. 0. 0.  0.     SO4:         (anions  3-20)
 0.    0.    0.   0.   0.    0.   0.   0.  0. 0. 0. 0. 0. 0. 0. 0. 0.         HSO4:        (anions  4-20)
 0.    .10   0.   0.   0.    0.   0.   0.  0. 0. 0. 0. 0. 0. 0. 0.           OH:          (anions  5-20)
-.04   0.    -.10 -.087 0.    0.   0.   0.  0. 0. 0. 0. 0. 0. 0.             HCO3:        (anions  6-20)
 0.    0.    0.   0.   0.    0.   0.   0.  0. 0. 0. 0. 0. 0.                 CO3:         (anions  7-20)
 0.    0.    0.   0.   0.    0.   0.   0.  0. 0. 0. 0. 0.                    B(OH)4:      (anions  8-20)
 0.    0.    0.   0.   0.    0.   0.   0.  0. 0. 0. 0.                       B3O3(OH)4:   (anions  9-20)
 0.    0.    0.   0.   0.    0.   0.   0.  0. 0. 0.                          B4O5(OH)4:   (anions 10-20)
 0.    0.    0.   0.   0.    0.   0.   0.  0. 0.                             Br:          (anions 11-20)
 0.    0.    0.   0.   0.    0.   0.   0.  0.                                Am(CO3)2-:   (anions 12-20)
 0.    0.    0.   0.   0.    0.   0.   0.                                   Am(CO3)3=-:  (anions 13-20)
 0.    0.    0.   0.   0.    0.   0.                                        ClO4-:       (anions 14-20)
 0.    0.    0.   0.   0.    0.                                             NpO2(OH)2-:  (anions 15-20)
 0.    0.    0.   0.   0.                                                  NpO2CO3-:    (anions 16-20)
 0.    0.    0.   0.                                                       NpO2(CO3)2=-:(anions 17-20)
 0.    0.    0.                                                            NPC3=5-:     (anions 18-20)
 0.    0.                                                                  H2PO4-:      (anions 19-20)
 0.                                                                        HPO4=:       (anions 20-20)


-.0018 -.010     .0  .0 -.003 .003 .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-K:20anions
 -.007 -.055     .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-Ca:
 -.012 -.015     .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-Mg:
    .0    .0     .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-MgOH:
  -.004   .0 -.0129 .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-H:
     .0    .0    .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-MgB(OH)4+
     .0    .0    .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-CaB(OH)4+
     .0    .0    .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-Am+++
     .0    .0    .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-AmCO3+
     .0    .0    .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-Th++++
     .0    .0    .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-UO2++
     .0    .0    .0  .0   .0   .0  .0 .0 .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 Na-NpO2++


-.025    .0     .0  .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -Ca:
-.022  -.048    .0  .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -Mg:
   .0     .0    .0  .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -MgOH:
-.011   .197 -.0265 .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -H :
   .0     .0    .0  .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -MgB(OH)4+
   .0     .0    .0  .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -CaB(OH)4+
   .0     .0    .0  .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -Am+++
   .0     .0    .0  .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -AmCO3+
   .0     .0    .0  .0  .0   .0  .0  .0  .0    .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 K -Th++++
```

Appendix I: Listing of HMW_NP_AM_RTEST.CHEMDAT and References Cited in Listing

```
   .0     .0     .0  .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 0 K -UO2++
   .0     .0     .0  .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0 0 0 0 0 K -NpO2++

-.012 .024  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-Mg:
   .0  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-MgOH:
-.015  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-H :
   .0  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-MgB(OH)4+
   .0  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-CaB(OH)4+
   .0  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-Am+++
   .0  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-AmCO3+
   .0  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-Th++++
   .0  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-UO2++
   .0  .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Ca-NpO2++

 .028 .0     .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-MgOH:
-.011 .0  -.0178 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-H :
   .0  .0     .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-MgB(OH)4+
   .0  .0     .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-CaB(OH)4+
   .0  .0     .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-Am+++
   .0  .0     .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-AmCO3+
   .0  .0     .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-Th++++
   .0  .0     .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-UO2++
   .0  .0     .0  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  .0 0 0 0 0 0 0 0 Mg-NpO2++

  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgOH-H :
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgOH-MgB(OH)4+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgOH-CaB(OH)4+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgOH-Am+++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgOH-AmCO3+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgOH-Th++++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgOH-UO2++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgOH-NpO2++

  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 H-MgB(OH)4+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 H-CaB(OH)4+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 H-Am+++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 H-AmCO3+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 H-Th++++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 H-UO2++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 H-NpO2++

  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgB(OH)4-CaB(OH)4+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgB(OH)4-Am+++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgB(OH)4-AmCO3+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgB(OH)4-Th++++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgB(OH)4-UO2++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 MgB(OH)4-NpO2++

  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 CaB(OH)4-Am+++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 CaB(OH)4-AmCO3+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 CaB(OH)4-Th++++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 CaB(OH)4-UO2++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 CaB(OH)4-NpO2++

  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 Am+++-AmCO3+
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 Am+++-Th++++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 Am+++-UO2++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 Am+++-NpO2++

  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 AmCO3+-Th++++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 AmCO3+-UO2++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 AmCO3+-NpO2++

  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 Th++++-UO2++
  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 Th++++-NpO2++

  .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0 UO2++-NpO2++

 .0014    .0 -.018 -.004  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-SO4:(Na,K,Ca,Mg,
 -.006    .0    .0   .0  .0 .013  .0  .0   .0   .0   .0   .0   .0   .0  Cl-HSO4:  MgOH,H,MgB(OH)3,
 -.006 -.006 -.025   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-OH:    CaB(OH)4,Am+++,
 -.015    .0    .0 -.096  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-HCO3:  AmCO3+,Th++++,
 .0085  .004    .0   .0   .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-CO3:   UO2++,NpO2+)
-.0073    .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-B(OH)4:
 -.024    .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-B3O3(OH)4:
   .026   .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-B4O5(OH)4:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-Br:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-Am(CO3)2:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-Am(CO3)3:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-C104-:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-NpO2(OH)2-:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-NpO2CO3-:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-NpO2(CO3)2=-:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-NpO2(CO3)3==-:
      .0 -.01   .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-H2PO4-:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-HPO4=:
      .0  .0    .0   .0  .0   .0  .0  .0   .0   .0   .0   .0   .0   .0  Cl-PO4=-:

-.0094 -.0677 .0 -.0425 .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-HSO4:
 -.009 -.050 .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-OH:
 -.005  .0    .0  -.161 .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-HCO3:
 -.005 -.009 .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-CO3:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-B(OH)4:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-B3O3(OH)4:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-B4O5(OH)4:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-Br:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-Am(CO3)2:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-Am(CO3)3:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-C104-:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-NpO2(OH)2-:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-NpO2CO3-:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-NpO2(CO3)2=-:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-NpO2(CO3)3==-:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-H2PO4-:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-HPO4=:
    .0    .0   .0    .0  .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  SO4-PO4=-:

   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-OH:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-HCO3-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-CO3=:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-B(OH)4-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-B3O3(OH)4:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-B4O5(OH)4:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-Br-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-Am(CO3)2-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-Am(CO3)2=-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-C104-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-NpO2(OH)2-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-NpO2CO3-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-NpO2(CO3)2=-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-NpO2(CO3)3==-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-H2PO4-:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-HPO4=:
   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HSO4-PO4=-:
```

```

   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-HCO3;
-.017 -.01  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-CO3;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-B(OH)4;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-B3O3(OH)4;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-B4O5(OH)4;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-Br;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-Am(CO3)2;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-Am(CO3)3;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-ClO4-;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-NpO2(OH)2-;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-NpO2CO3-;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-NpO2(CO3)2=-;
   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  OH-PO4=-;

 .002 .012  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-CO3;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-B(OH)4;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-B3O3(OH)4;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-B4O5(OH)4;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-Br;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-Am(CO3)2;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-Am(CO3)3;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-ClO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-NpO2(OH)2-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-PO4=-;

 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-B(OH)4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-B3O3(OH)4;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-B4O5(OH)4;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-Br;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-Am(CO3)2;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-Am(CO3)3;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-ClO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-NpO2(OH)2-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-PO4=-;

 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-B3O3(OH)4;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-B4O5(OH)4;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-Br;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-Am(CO3)2;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-Am(CO3)3;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-ClO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-NpO2(OH)2-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-PO4=-;

 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-B4O5(OH)4;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-Br;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-Am(CO3)2;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-Am(CO3)3;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-ClO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-NpO2(OH)2-
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-PO4=-;

 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-Br;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-Am(CO3)2;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-Am(CO3)3;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-ClO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-NPO2(OH)2-
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4-PO4=-;

 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-Am(CO3)2;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-Am(CO3)3;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-ClO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-NpO2(OH)2-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-PO4=-;

 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-Am(CO3)3;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-ClO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-NpO2(OH)2-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-PO4=-;

 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)3-ClO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)3-NpO2(OH)2-
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)3-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)3-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)3-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)3-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)3-HPO4=;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)3-PO4=-;

 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  ClO4-NpO2(OH)2-
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  ClO4-NpO2CO3-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  ClO4-NpO2(CO3)2=-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  ClO4-NpO2(CO3)3==-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  ClO4-H2PO4-;
 .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  ClO4-HPO4=;
```

Appendix I: Listing of HMW_NP_AM_RTEST.CHEMDAT and References Cited in Listing

```
726     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  ClO4-PO4=-;
727
728     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(OH)2--NpO2CO3-;
729     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(OH)2--NpO2(CO3)2=-;
730     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(OH)2--NpO2(CO3)3=3-;
731     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(OH)2-H2PO4-;
732     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(OH)2-HPO4=;
733     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(OH)2-PO4=-;
734
735     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2CO3-NpO2(CO3)2=-;
736     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2CO3-NpO2(CO3)3=3-;
737     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2CO3-H2PO4-;
738     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2CO3-HPO4=;
739     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2CO3-PO4=-;
740
741     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2-NpO2(CO3)3=3-;
742     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2-H2PO4-;
743     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2-HPO4=;
744     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2-PO4=-;
745
746     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(CO3)3-H2PO4-;
747     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(CO3)3-HPO4=;
748     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  NpO2(CO3)3-PO4=-;
749
750     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  H2PO4-HPO4=;
751     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  H2PO4-PO4=-;
752
753     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  HPO4-PO4=-;
754
755    .100 .051  .183 .183 .0   .0   .0   .0   .0   .0   .0   .0   .0    CO2-Cations     NMW84
756      .0   .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0    CaCO3-Cations   NMW84
757      .0   .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0    MgCO3-Cations   NMW84
758   -.097 -.14    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0    B(OH)3-Cations  FW86
759      .0   .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0    NpO2OH-Cations
760      .0 -.07    .0   .0  .0  .29   .0   .0   .0   .0   .0   .0   .0    H3PO4-Cations   PS76
761
762   -.005 .097 -.003    .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0   0  0  0  CO2-Anions     NMW84
763      .0   .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0   0  0  0  CaCO3-Anions   NMW84
764      .0   .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0   0  0  0  MgCO3-Anions   NMW84
765     .091 .018    .0   .0  .0   .0   .0 -.20   .0   .0   .0   .0   .0  0  0  0  0   0  0  0  B(OH)3-Anions  FW86
766      .0   .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0   0  0  0  NpO2OH-Anions
767      .0   .0    .0   .0  .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  -.4  0  0  H3PO4-Anions   PS76
768
769    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  CO2-Cation-Anion
770    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  (Cations down, Anions across)
771    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
772    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
773    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
774    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
775    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
776    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
777    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
778    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
779    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
780    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
781    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
782
783    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  CaCO3-Cation-Anion
784    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
785    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
786    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
787    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
788    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
789    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
790    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
791    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
792    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
793    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
794    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
795    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
796
797    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  MgCO3-Cation-Anion
798    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
799    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
800    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
801    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
802    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
803    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
804    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
805    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
806    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
807    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
808    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
809    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
810
811    .0     .046 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  B(OH)3-Cation-Anion FW86
812    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  (Cations down, Anions across)
813    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
814    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
815    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
816   -.0102 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
817    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
818    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
819    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
820    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
821    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
822    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
823    .0     .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
824
825    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  NpO2OH(aq)-Cation-Anion
826    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
827    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
828    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
829    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
830    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
831    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
832    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
833    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
834    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
835    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
836    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
837    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
838
839    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0  H3PO4-Cation-Anion
840    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
841    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
842    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
843    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
844    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
845    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
846    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
847    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
848    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
849    .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0  0  0  0  0
```

Appendix I: Listing of HMW_NP_AM_RTEST.CHEMDAT and References Cited in Listing

```
 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0

  2   3   4   5   6   7      Na+          K+          Ca++        Mg++        MgOH+  H+              cation map ELMAP(1,)
 22  21  43  44  49  50      MgB(OH)4+    CaB(OH)4+   Am+++       AmCO3+      Th++++ UO2++
 37                          NpO2+

  8   9  10  11  12  13      Cl-          SO4=        HSO4-       OH-         HCO3-       CO3=        anion map ELMAP(2,)
 18  19  20  23  45  46      B(OH)4-      BJO3(OH)6-  B4O5(OH)4=  Br-        Am(CO3)2-   Am(CO3)3=-
 24  39  40  41  42  34      ClO4-        NpO2(OH)2-  NpO2CO3-     NpO2(CO3)2=- NpO2(CO3)3=== H2PO4-
 35  36                      HPO4=        PO4=-

 14  15  16  17  38  33      CO2(aq)      CaCO3(aq)   MgCO3(aq)   B(OH)3(aq)  NpO2OH(aq)  H3PO4(aq)   neutral map ELMAP(3,)
'nEQUALACT' 0

2 (Oxygen)
'nREDOX' 0
'nIONEX' 0 0 'nMF'


FRER89 ==  Felmy, Rai, Schramke, and Ryan (1989) RCA 48 pp.29-35
FRF90  ==  Felmy, Rai, and Fulton (1990) RCA 50 pp.193-204
PS76   ==  Pitzer and Silvester (1976) J Soln Chem 5#4 pp.269-278
P91    ==  Pitzer (1991) CRC Handbook, Activity Coef in Electrolyte Solns
RFF92  ==  Rai, Felmy, and Fulton (1992)  RCA 56 pp.7-14
RFFR92 ==  Rai, Felmy, Fulton, and Ryan (1992) RCA 58/59 pp.9-16
RFF94  ==  Rai, Felmy, and Fulton (1994)
RRFF94 ==  Rao, Rai, Felmy, and Fulton (1994) SAND94-1948J for RCA

NR94   ==  Novak and Roberts (1994) SAND94-xxxx MRS/Kyoto
HMW84  ==  Harvie, Moller, Weare (1984) GCA 48 pp.723-751
FW86   ==  Felmy and Weare (1986) GCA 50 pp.2771-2783
```

I.2 References Cited in Listing

Felmy, A.R., D. Rai, and R.W. Fulton. 1990. "The Solubility of AmOHCO3(c) and the Aqueous Thermodynamics of the System Na+-Am3+-HCO_3^--OH—H2O." Radiochimica Acta vol. 50: 193-240.

Felmy, A.R., D. Rai, J.A. Schramke, and J.L. Ryan. 1989. "The Solubility of Plutonium Hydroxide in Dilute Solution and in High-Ionic-Strength Chloride Brines." *Radiochimica Acta* vol. 48: 29-35.

Felmy, A.R., and J.H. Weare. 1986. "The Prediction of Borate Mineral Equilibria in Natural Waters: Application to Searles Lake, California." *Geochimica et Cosmochimica Acta* vol. 50: 2771-2783.

Harvie, C.E., N. Møller, and J.H. Weare. 1984. "The Prediction of Mineral Solubilities in Natural Waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O System to High Ionic Strength at 25_C." *Geochimica et Cosmochimica Acta* vol. 48: 723-751.

Novak, C.F., and K.E. Roberts. 1994. *Thermodynamic Modeling of Neptunium(V) Solubility in Na-CO3-HCO3-Cl-ClO4-H-OH-H2O Electrolytes*. SAND94-0805C. Albuquerque, New Mexico: Sandia National Laboratories.

Pitzer, K.S. 1991. *Activity Coefficients in Electrolyte Solutions*. Boca Raton, Florida: CRC Press.

Pitzer, K.S., and L.F. Silvester. 1976. "Thermodynamics of Electrolytes. VI. Weak Electrolytes Including H3PO4." *Journal of Solution Chemistry* vol. 5: 269-278.

Rai, D., A.R. Felmy, and R.W. Fulton. 1992a. "Solubility and Ion Activity Product of $AmPO_4 \cdot xH_2O(am)$." *Radiochimica Acta* vol. 56: 7-14.

Rai, D., A.R. Felmy, and R.W. Fulton. 1994. "The Nd^{3+} and Am^{3+} Ion Interactions with SO_4^{2-} and their Influence on $NdPO_4(c)$ Solubility." *Journal of Solution Chemistry*. submitted June 1994.

Rai, D., A.R. Felmy, R.W. Fulton, and J.L. Ryan. 1992b. "Aqueous Chemistry of Nd in Borosilicate-Glass/Water Systems." *Radiochimica Acta* vol. 58/59: 9-16.

Rao, L., D. Rai, A.R. Felmy, and RW. Fulton. 1994. "Solubility of $NaNd(CO_3)_2 \cdot 6H_2O$ in Concentrated Sodium Carbonate and Sodium Bicarbonate Solutions." *Radiochimica Acta* vol. 24, no. 2: 879-895.

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

See Table 11 for explanation of this listing.

```
CHEMDAT  file name is U1:[SCBABB.FMT.UM]FMT_HMW_NP_AM_RTEST.CHEMDAT;1
 Temperature is Hard Coded as 298.15K
 [.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs                FMT V2.3
 DATABASE:  HMW84/PM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

 Accuracy of reactions is              1.0000E-06
 Minimum elemental abundance is        1.0000E-18
 Number of Aqueous Species is           50


 Species Order for Pitzer Parameters

 Cations    13

 Na+              K+               Ca++             Mg++             MgOH+            H+
 MgB(OH)4+        CaB(OH)4+        Am+++            AmCO3+           Th++++           UO2++
 NpO2+

 Anions     20

 Cl-              SO4=             HSO4-            OH-              HCO3-            CO3=
 B(OH)4-          B3O3(OH)4-       B4O5(OH)4=       Br-              Am(CO3)2-        Am(CO3)3=-
 ClO4-            pe NpO2(OH)2-    NpO2CO3-         NpO2(CO3)2=-     NpO2(CO3)3=-=    H2PO4-
 HPO4=            PO4=-

 Neutral    6

 CO2(aq)          CaCO3(aq)        MgCO3(aq)        B(OH)3(aq)       NpO2OH(aq)       H3PO4(aq)


 Cation-Anion Binary Interection Parameters

 Cation     Anion            Beta(0)     Beta(1)     Beta(2)     Cphi      Alpha-Values
 Na+        Cl-              0.07650     0.26440     0.00000     0.00127   (2.0,12) 1-1,1-2,2-3
 Na+        SO4=             0.01958     1.11300     0.00000     0.00497   (2.0,12) 1-1,1-2,2-3
 Na+        HSO4-            0.04540     0.39800     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        OH-              0.08640     0.25300     0.00000     0.00440   (2.0,12) 1-1,1-2,2-3
 Na+        HCO3-            0.02770     0.04110     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        CO3=             0.01990     1.38900     0.00000     0.00440   (2.0,12) 1-1,1-2,2-3
 Na+        B(OH)4-          -0.04270    0.08900     0.00000     0.01140   (2.0,12) 1-1,1-2,2-3
 Na+        B3O3(OH)4-       -0.05600    -0.91000    0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        B4O5(OH)4=       -0.11000    -0.40000    0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        Br-              0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        Am(CO3)2-        0.00000     -8.37000    0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        Am(CO3)3=-       -0.94000    8.10000     0.00000     0.41800   (2.0,12) 1-1,1-2,2-3
 Na+        ClO4-            0.05540     0.27550     0.00000     -0.00118  (2.0,12) 1-1,1-2,2-3
 Na+        NpO2(OH)2-       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        NpO2CO3-         0.16100     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        NpO2(CO3)2=-     0.40700     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        NpO2(CO3)3=-=    1.97000     16.00000    0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Na+        H2PO4-           -0.05330    0.03960     0.00000     0.00795   (2.0,12) 1-1,1-2,2-3
 Na+        HPO4=            -0.05830    1.46600     0.00000     0.02940   (2.0,12) 1-1,1-2,2-3
 Na+        PO4=-            0.17810     3.85100     0.00000     -0.05154  (2.0,12) 1-1,1-2,2-3

 K+         Cl-              0.04835     0.21220     0.00000     -0.00084  (2.0,12) 1-1,1-2,2-3
 K+         SO4=             0.04995     0.77930     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         HSO4-            -0.00030    0.17350     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         OH-              0.12980     0.32000     0.00000     0.00410   (2.0,12) 1-1,1-2,2-3
 K+         HCO3-            0.02960     -0.01300    0.00000     -0.00800  (2.0,12) 1-1,1-2,2-3
 K+         CO3=             0.14880     1.43000     0.00000     -0.00150  (2.0,12) 1-1,1-2,2-3
 K+         B(OH)4-          0.03500     0.14000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         B3O3(OH)4-       -0.13000    0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         B4O5(OH)4=       -0.02200    0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         Br-              0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         Am(CO3)2-        0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         Am(CO3)3=-       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         ClO4-            0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         NpO2(OH)2-       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         NpO2CO3-         0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         NpO2(CO3)2=-     0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         NpO2(CO3)3=-=    0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         H2PO4-           -0.06780    -0.10420    0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 K+         HPO4=            0.02480     1.27400     0.00000     0.01640   (2.0,12) 1-1,1-2,2-3
 K+         PO4=-            0.37290     3.97200     0.00000     -0.08680  (2.0,12) 1-1,1-2,2-3

 Ca++       Cl-              0.31590     1.61400     0.00000     -0.00034  (2.0,12) 1-1,1-2,2-3
 Ca++       SO4=             0.20000     3.19730     -54.24000   0.00000   (1.4,12) 2-2
 Ca++       HSO4-            0.21450     2.53000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       OH-              -0.17470    -0.23030    -5.72000    0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       HCO3-            0.40000     2.97700     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       CO3=             0.00000     0.00000     0.00000     0.00000   (1.4,12) 2-2
 Ca++       B(OH)4-          0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       B3O3(OH)4-       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       B4O5(OH)4=       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       Br-              0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       Am(CO3)2-        0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       Am(CO3)3=-       0.00000     0.00000     0.00000     0.00000   (1.4,50) 2-(n>2)
 Ca++       ClO4-            0.45110     1.75600     0.00000     -0.00500  (2.0,12) 1-1,1-2,2-3
 Ca++       NpO2(OH)2-       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       NpO2CO3-         0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       NpO2(CO3)2=-     0.00000     0.00000     0.00000     0.00000   (1.4,50) 2-(n>2)
 Ca++       NpO2(CO3)3=-=    0.00000     0.00000     0.00000     0.00000   (1.4,50) 2-(n>2)
 Ca++       H2PO4-           0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Ca++       HPO4=            0.00000     0.00000     0.00000     0.00000   (1.4,12) 2-2
 Ca++       PO4=-            0.00000     0.00000     0.00000     0.00000   (1.4,50) 2-(n>2)

 Mg++       Cl-              0.35235     1.68150     0.00000     0.00519   (2.0,12) 1-1,1-2,2-3
 Mg++       SO4=             0.22100     3.34300     -37.23000   0.02500   (1.4,12) 2-2
 Mg++       HSO4-            0.47460     1.72900     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       OH-              0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       HCO3-            0.32900     0.60720     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       CO3=             0.00000     0.00000     0.00000     0.00000   (1.4,12) 2-2
 Mg++       B(OH)4-          0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       B3O3(OH)4-       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       B4O5(OH)4=       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       Br-              0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       Am(CO3)2-        0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       Am(CO3)3=-       0.00000     0.00000     0.00000     0.00000   (1.4,50) 2-(n>2)
 Mg++       ClO4-            0.49610     2.00800     0.00000     0.00958   (2.0,12) 1-1,1-2,2-3
 Mg++       NpO2(OH)2-       0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
 Mg++       NpO2CO3-         0.00000     0.00000     0.00000     0.00000   (2.0,12) 1-1,1-2,2-3
```

115	Mg++	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
116	Mg++	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
117	Mg++	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
118	Mg++	HPO4=	0.00000	0.00000	0.00000	0.00000	(1,4,12)	2-2
119	Mg++	PO4---	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
120								
121	MgOH+	Cl-	-0.10000	1.65800	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
122	MgOH+	SO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
123	MgOH+	HSO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
124	MgOH+	OH-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
125	MgOH+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
126	MgOH+	CO3=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
127	MgOH+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
128	MgOH+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
129	MgOH+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
130	MgOH+	Br-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
131	MgOH+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
132	MgOH+	Am(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
133	MgOH+	ClO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
134	MgOH+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
135	MgOH+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
136	MgOH+	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
137	MgOH+	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
138	MgOH+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
139	MgOH+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
140	MgOH+	PO4---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
141								
142	H+	Cl-	0.17750	0.29450	0.00000	0.00080	(2,0,12)	1-1,1-2,1-3
143	H+	SO4=	0.02980	0.00000	0.00000	0.04380	(2,0,12)	1-1,1-2,1-3
144	H+	HSO4-	0.20650	0.55560	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
145	H+	OH-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
146	H+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
147	H+	CO3=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
148	H+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
149	H+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
150	H+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
151	H+	Br-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
152	H+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
153	H+	Am(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
154	H+	ClO4-	0.17470	0.29310	0.00000	0.00819	(2,0,12)	1-1,1-2,1-3
155	H+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
156	H+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
157	H+	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
158	H+	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
159	H+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
160	H+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
161	H+	PO4---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
162								
163	MgB(OH)4+	Cl-	0.16000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
164	MgB(OH)4+	SO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
165	MgB(OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
166	MgB(OH)4+	OH-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
167	MgB(OH)4+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
168	MgB(OH)4+	CO3=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
169	MgB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
170	MgB(OH)4+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
171	MgB(OH)4+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
172	MgB(OH)4+	Br-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
173	MgB(OH)4+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
174	MgB(OH)4+	Am(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
175	MgB(OH)4+	ClO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
176	MgB(OH)4+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
177	MgB(OH)4+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
178	MgB(OH)4+	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
179	MgB(OH)4+	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
180	MgB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
181	MgB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
182	MgB(OH)4+	PO4---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
183								
184	CaB(OH)4+	Cl-	0.12000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
185	CaB(OH)4+	SO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
186	CaB(OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
187	CaB(OH)4+	OH-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
188	CaB(OH)4+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
189	CaB(OH)4+	CO3=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
190	CaB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
191	CaB(OH)4+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
192	CaB(OH)4+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
193	CaB(OH)4+	Br-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
194	CaB(OH)4+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
195	CaB(OH)4+	Am(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
196	CaB(OH)4+	ClO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
197	CaB(OH)4+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
198	CaB(OH)4+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
199	CaB(OH)4+	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
200	CaB(OH)4+	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
201	CaB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
202	CaB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
203	CaB(OH)4+	PO4---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
204								
205	Am+++	Cl-	0.61170	5.40100	0.00000	-0.02840	(2,0,12)	1-1,1-2,1-3
206	Am+++	SO4=	3.03980	0.00000	-2500.00000	0.00000	(1,4,50)	2-(n>2)
207	Am+++	HSO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
208	Am+++	OH-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
209	Am+++	HCO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
210	Am+++	CO3=	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
211	Am+++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
212	Am+++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
213	Am+++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
214	Am+++	Br-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
215	Am+++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
216	Am+++	Am(CO3)3---	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
217	Am+++	ClO4-	0.80300	5.35000	0.00000	-0.00480	(2,0,12)	1-1,1-2,1-3
218	Am+++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
219	Am+++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
220	Am+++	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
221	Am+++	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
222	Am+++	H2PO4-	0.00000	0.00000	-92.90000	0.00000	(2,0,12)	1-1,1-2,1-3
223	Am+++	HPO4=	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
224	Am+++	PO4---	0.00000	0.00000	0.00000	0.00000	(1,4,50)	2-(n>2)
225								
226	AmCO3+	Cl-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
227	AmCO3+	SO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
228	AmCO3+	HSO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
229	AmCO3+	OH-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
230	AmCO3+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
231	AmCO3+	CO3=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
232	AmCO3+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
233	AmCO3+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
234	AmCO3+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
235	AmCO3+	Br-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
236	AmCO3+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
237	AmCO3+	Am(CO3)3---	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3
238	AmCO3+	ClO4-	0.00000	0.00000	0.00000	0.00000	(2,0,12)	1-1,1-2,1-3

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

```
239 AmCO3+          NpO2(OH)2-          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
240 AmCO3+          NpO2CO3-            0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
241 AmCO3+          NpO2(CO3)2+-        0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
242 AmCO3+          NpO2(CO3)3+++       0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
243 AmCO3+          H2PO4-              0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
244 AmCO3+          HPO4+               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
245 AmCO3+          PO4+-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
246
247 Th++++          Cl-                 0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
248 Th++++          SO4+                0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
249 Th++++          HSO4-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
250 Th++++          OH-                 0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
251 Th++++          HCO3-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
252 Th++++          CO3+                0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
253 Th++++          B(OH)4-             0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
254 Th++++          B3O3(OH)4-          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
255 Th++++          B4O5(OH)4+          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
256 Th++++          Br-                 0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
257 Th++++          Am(CO3)2-           0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
258 Th++++          Am(CO3)3+-          0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
259 Th++++          ClO4-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
260 Th++++          NpO2(OH)2-          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
261 Th++++          NpO2CO3-            0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
262 Th++++          NpO2(CO3)2+-        0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
263 Th++++          NpO2(CO3)3+++       0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
264 Th++++          H2PO4-              0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
265 Th++++          HPO4+               0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
266 Th++++          PO4+-               0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
267
268 UO2++           Cl-                 0.42740   1.64400   0.00000  -0.03686  (2.0,12) 1-1,1-2,1-3
269 UO2++           SO4+                0.32200   1.82700   0.00000  -0.01760  (1.4,12) 2-2
270 UO2++           HSO4-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
271 UO2++           OH-                 0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
272 UO2++           HCO3-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
273 UO2++           CO3+                0.00000   0.00000   0.00000   0.00000  (1.4,12) 2-2
274 UO2++           B(OH)4-             0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
275 UO2++           B3O3(OH)4-          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
276 UO2++           B4O5(OH)4+          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
277 UO2++           Br-                 0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
278 UO2++           Am(CO3)2-           0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
279 UO2++           Am(CO3)3+-          0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
280 UO2++           ClO4-               0.61130   2.14400   0.00000   0.02168  (2.0,12) 1-1,1-2,1-3
281 UO2++           NpO2(OH)2-          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
282 UO2++           NpO2CO3-            0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
283 UO2++           NpO2(CO3)2+-        0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
284 UO2++           NpO2(CO3)3+++       0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
285 UO2++           H2PO4-              0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
286 UO2++           HPO4+               0.00000   0.00000   0.00000   0.00000  (1.4,12) 2-2
287 UO2++           PO4+-               0.00000   0.00000   0.00000   0.00000  (1.4,50) 2-(n>2)
288
289 NpO2+           Cl-                 0.16900   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
290 NpO2+           SO4+                0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
291 NpO2+           HSO4-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
292 NpO2+           OH-                 0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
293 NpO2+           HCO3-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
294 NpO2+           CO3+                0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
295 NpO2+           B(OH)4-             0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
296 NpO2+           B3O3(OH)4-          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
297 NpO2+           B4O5(OH)4+          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
298 NpO2+           Br-                 0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
299 NpO2+           Am(CO3)2-           0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
300 NpO2+           Am(CO3)3+-          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
301 NpO2+           ClO4-               0.31200   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
302 NpO2+           NpO2(OH)2-          0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
303 NpO2+           NpO2CO3-            0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
304 NpO2+           NpO2(CO3)2+-        0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
305 NpO2+           NpO2(CO3)3+++       0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
306 NpO2+           H2PO4-              0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
307 NpO2+           HPO4+               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
308 NpO2+           PO4+-               0.00000   0.00000   0.00000   0.00000  (2.0,12) 1-1,1-2,1-3
309
310 Cation-Cation Ternary Interactions:  theta(c1,c2)
311
312                     K+          Ca++        Mg++        MgOH+       H+          MgB(OH)4+   CaB(OH)4+   Am+++       AmCO3+      Th++++
313 Na+                 -0.01200    0.07000     0.07000     0.00000     0.03600     0.00000     0.00000     0.00000     0.00000     0.00000
314                     UO2++       NpO2+
315 Na+                 0.00000     0.00000
316
317                     Ca++        Mg++        MgOH+       H+          MgB(OH)4+   CaB(OH)4+   Am+++       AmCO3+      Th++++      UO2++
318 K+                  0.03200     0.00000     0.00000     0.00500     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
319                     NpO2+
320 K+                  0.00000
321
322                     Mg++        MgOH+       H+          MgB(OH)4+   CaB(OH)4+   Am+++       AmCO3+      Th++++      UO2++       NpO2+
323 Ca++                0.00700     0.00000     0.09200     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
324
325                     MgOH+       H+          MgB(OH)4+   CaB(OH)4+   Am+++       AmCO3+      Th++++      UO2++       NpO2+
326 Mg++                0.00000     0.10000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
327
328                     H+          MgB(OH)4+   CaB(OH)4+   Am+++       AmCO3+      Th++++      UO2++       NpO2+
329 MgOH+               0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
330
331                     MgB(OH)4+   CaB(OH)4+   Am+++       AmCO3+      Th++++      UO2++       NpO2+
332 H+                  0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
333
334                     CaB(OH)4+   Am+++       AmCO3+      Th++++      UO2++       NpO2+
335 MgB(OH)4+           0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
336
337                     Am+++       AmCO3+      Th++++      UO2++       NpO2+
338 CaB(OH)4+           0.00000     0.00000     0.00000     0.00000     0.00000
339
340                     AmCO3+      Th++++      UO2++       NpO2+
341 Am+++               0.00000     0.00000     0.00000     0.00000
342
343                     Th++++      UO2++       NpO2+
344 AmCO3+              0.00000     0.00000     0.00000
345
346                     UO2++       NpO2+
347 Th++++              0.00000     0.00000
348
349                     NpO2+
350 UO2++               0.00000
351
352
353 Anion-Anion Ternary Interactions:  theta(a1,a2)
354
355                     SO4+        HSO4-       OH-         HCO3-       CO3+        B(OH)4-     B3O3(OH)4-  B4O5(OH)4+  Br-         Am(CO3)2-
356 Cl-                 0.02000     -0.00600    -0.05000    0.03000     -0.02000    -0.06500    0.12000     0.07400     0.00000     0.00000
357                     Am(CO3)3+-  ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4+       PO4+-
358 Cl-                 0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.10000     0.00000     0.00000
359
360                     HSO4-       OH-         HCO3-       CO3+        B(OH)4-     B3O3(OH)4-  B4O5(OH)4+  Br-         Am(CO3)2-   Am(CO3)3+-
361 SO4+                0.00000     -0.01300    0.01000     0.02000     -0.01200    0.10000     0.12000     0.00000     0.00000     0.00000
362                     ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4+       PO4+-
```

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

```
353 SO4=          0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
354
355                OH-       HCO3-     CO3=      B(OH)4-   B3O3(OH)4- B4O5(OH)4= Br-       Am(CO3)2- Am(CO3)3=- ClO4-
356 HSO4-         0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
357                NpO2(OH)2- NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
358 HSO4-         0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
359
360                HCO3-     CO3=      B(OH)4-   B3O3(OH)4- B4O5(OH)4= Br-       Am(CO3)2- Am(CO3)3=- ClO4-     NpO2(OH)2-
361 OH-           0.00000   0.10000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
362                NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
363 OH-           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
364
365                CO3=      B(OH)4-   B3O3(OH)4- B4O5(OH)4= Br-       Am(CO3)2- Am(CO3)3=- ClO4-     NpO2(OH)2- NpO2CO3-
366 HCO3-         -0.04000   0.00000  -0.10000  -0.08700   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
367                NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
368 HCO3-         0.00000   0.00000   0.00000   0.00000   0.00000
369
370                B(OH)4-   B3O3(OH)4- B4O5(OH)4= Br-       Am(CO3)2- Am(CO3)3=- ClO4-     NpO2(OH)2- NpO2CO3-  NpO2(CO3)2
371 CO3=          0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
372                NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
373 CO3=          0.00000   0.00000   0.00000   0.00000
374
375                B3O3(OH)4- B4O5(OH)4= Br-       Am(CO3)2- Am(CO3)3=- ClO4-     NpO2(OH)2- NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3
376 B(OH)4-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
377                H2PO4-    HPO4=     PO4=-
378 B(OH)4-       0.00000   0.00000   0.00000
379
380                B4O5(OH)4= Br-       Am(CO3)2- Am(CO3)3=- ClO4-     NpO2(OH)2- NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-
381 B3O3(OH)4-    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
382                HPO4=     PO4=-
383 B3O3(OH)4-    0.00000   0.00000
384
385                Br-       Am(CO3)2- Am(CO3)3=- ClO4-     NpO2(OH)2- NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=
386 B4O5(OH)4=    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
387                PO4=-
388 B4O5(OH)4=    0.00000
389
390                Am(CO3)2- Am(CO3)3=- ClO4-     NpO2(OH)2- NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
391 Br-           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
392
393
394
395                Am(CO3)3=- ClO4-     NpO2(OH)2- NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
396 Am(CO3)2-     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
397
398
399
400                ClO4-     NpO2(OH)2- NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
401 Am(CO3)3=-     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
402
403                NpO2(OH)2- NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
404 ClO4-         0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
405
406                NpO2CO3-  NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
407 NpO2(OH)2-    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
408
409                NpO2(CO3)2 NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
410 NpO2CO3-      0.00000   0.00000   0.00000   0.00000   0.00000
411
412                NpO2(CO3)3 H2PO4-    HPO4=     PO4=-
413 NpO2(CO3)2=-   0.00000   0.00000   0.00000   0.00000
414
415                H2PO4-    HPO4=     PO4=-
416 NpO2(CO3)3=-=  0.00000   0.00000   0.00000
417
418                HPO4=     PO4=-
419 H2PO4-        0.00000   0.00000
420
421
422 HPO4=          0.00000
423
424
425
426
427
428
429
430
431 Cation-Cation-Anion Ternary Interactions: psi(,,,)
432
433                -         Cl-       SO4=      HSO4-     OH-       HCO3-     CO3=      B(OH)4-   B3O3(OH)4 B4O5(OH)4 Br-
434 Na+           K+        -0.00180  -0.01000  0.00000   0.00000   -0.00300  0.00100   0.00000   0.00000   0.00000   0.00000
435 Na+           Ca++      -0.00700  -0.05500  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
436 Na+           Mg++      -0.01200  -0.01500  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
437 Na+           MgOH+      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
438 Na+           H+        -0.00400   0.00000 -0.01290   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
439 Na+           MgB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
440 Na+           CaB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
441 Na+           Am+++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
442 Na+           AmCO3+     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
443 Na+           Th++++     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
444 Na+           UO2++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
445 Na+           NpO2+      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
446 K+            Ca++      -0.03500   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
447 K+            Mg++      -0.02200  -0.04800  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
448 K+            MgOH+      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
449 K+            H+        -0.01100   0.19700 -0.02650   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
450 K+            MgB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
451 K+            CaB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
452 K+            Am+++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
453 K+            AmCO3+     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
454 K+            Th++++     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
455 K+            UO2++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
456 K+            NpO2+      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
457 Ca++          Mg++      -0.01200   0.02400  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
458 Ca++          MgOH+      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
459 Ca++          H+        -0.01500   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
460 Ca++          MgB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
461 Ca++          CaB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
462 Ca++          Am+++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
463 Ca++          AmCO3+     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
464 Ca++          Th++++     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
465 Ca++          UO2++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
466 Ca++          NpO2+      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
467 Mg++          MgOH+      0.02800   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
468 Mg++          H+        -0.01100   0.00000 -0.01780   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
469 Mg++          MgB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
470 Mg++          CaB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
471 Mg++          Am+++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
472 Mg++          AmCO3+     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
473 Mg++          Th++++     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
474 Mg++          UO2++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
475 Mg++          NpO2+      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
476 MgOH+         H+         0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
477 MgOH+         MgB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
478 MgOH+         CaB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
479 MgOH+         Am+++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
480 MgOH+         AmCO3+     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
481 MgOH+         Th++++     0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
482 MgOH+         UO2++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
483 MgOH+         NpO2+      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
484 H+            MgB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
485 H+            CaB(OH)4+  0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
486 H+            Am+++      0.00000   0.00000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
```

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

487	H+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
488	H+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
489	H+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
490	H+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
491	MgB(OH)4+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
492	MgB(OH)4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
493	MgB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
494	MgB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
495	MgB(OH)4+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
496	MgB(OH)4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
497	CaB(OH)4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
498	CaB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
499	CaB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
500	CaB(OH)4+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
501	CaB(OH)4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
502	Am+++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
503	Am+++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
504	Am+++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
505	Am+++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
506	AmCO3+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
507	AmCO3+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
508	AmCO3+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
509	Th++++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
510	Th++++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
511	UO2++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
512												
513			Am(CO3)2-	Am(CO3)3-3	C104-	NpO2(OH)2	NpO2CO3-	NpO2(CO3)	NpO2(CO3)2	H2PO4-	HPO4+	PO4+-
514	Na+	K+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
515	Na+	Ca++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
516	Na+	Mg++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
517	Na+	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
518	Na+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
519	Na+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
520	Na+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
521	Na+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
522	Na+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
523	Na+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
524	Na+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
525	Na+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
526	K+	Ca++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
527	K+	Mg++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
528	K+	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
529	K+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
530	K+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
531	K+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
532	K+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
533	K+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
534	K+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
535	K+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
536	K+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
537	Ca++	Mg++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
538	Ca++	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
539	Ca++	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
540	Ca++	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
541	Ca++	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
542	Ca++	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
543	Ca++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
544	Ca++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
545	Ca++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
546	Ca++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
547	Mg++	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
548	Mg++	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
549	Mg++	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
550	Mg++	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
551	Mg++	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
552	Mg++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
553	Mg++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
554	Mg++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
555	Mg++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
556	MgOH+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
557	MgOH+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
558	MgOH+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
559	MgOH+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
560	MgOH+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
561	MgOH+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
562	MgOH+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
563	MgOH+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
564	H+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
565	H+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
566	H+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
567	H+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
568	H+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
569	H+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
570	H+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
571	MgB(OH)4+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
572	MgB(OH)4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
573	MgB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
574	MgB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
575	MgB(OH)4+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
576	MgB(OH)4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
577	CaB(OH)4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
578	CaB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
579	CaB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
580	CaB(OH)4+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
581	CaB(OH)4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
582	Am+++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
583	Am+++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
584	Am+++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
585	Am+++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
586	AmCO3+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
587	AmCO3+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
588	AmCO3+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
589	Th++++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
590	Th++++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
591	UO2++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
592												
593	Anion-Anion-Cation Ternary Interactions: psi(...)											
594												
595			Na+	K+	Ca++	Mg++	MgOH+	H+	MgB(OH)4+	CaB(OH)4+	Am+++	AmCO3+
596	Cl-	SO4+	0.00140	0.00000	-0.01800	-0.00400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
597	Cl-	HSO4-	-0.00600	0.00000	0.00000	0.00000	0.00000	0.01100	0.00000	0.00000	0.00000	0.00000
598	Cl-	OH-	-0.00600	-0.00600	-0.02500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
599	Cl-	HCO3-	-0.01500	0.00000	0.00000	-0.09600	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
600	Cl-	CO3+	0.00850	0.00400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
601	Cl-	B(OH)4-	-0.00730	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
602	Cl-	B3O3(OH)4-	-0.02400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
603	Cl-	B4O5(OH)4+	0.02600	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
604	Cl-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
605	Cl-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
606	Cl-	Am(CO3)3+-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
607	Cl-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
608	Cl-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
609	Cl-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
610	Cl-	NpO2(CO3)2+-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

611	Cl-	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
612	Cl-	H2PO4-	0.00000	-0.01000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
613	Cl-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
614	Cl-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
615	SO4=	HSO4-	-0.00940	-0.06770	0.00000	-0.04350	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
616	SO4=	OH-	-0.00900	-0.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
617	SO4=	HCO3-	-0.00500	0.00000	0.00000	-0.16100	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
618	SO4=	CO3=	-0.00500	-0.00900	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
619	SO4=	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
620	SO4=	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
621	SO4=	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
622	SO4=	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
623	SO4=	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
624	SO4=	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
625	SO4=	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
626	SO4=	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
627	SO4=	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
628	SO4=	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
629	SO4=	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
630	SO4=	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
631	SO4=	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
632	SO4=	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
633	HSO4-	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
634	HSO4-	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
635	HSO4-	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
636	HSO4-	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
637	HSO4-	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
638	HSO4-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
639	HSO4-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
640	HSO4-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
641	HSO4-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
642	HSO4-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
643	HSO4-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
644	HSO4-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
645	HSO4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
646	HSO4-	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
647	HSO4-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
648	HSO4-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
649	HSO4-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
650	OH-	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
651	OH-	CO3=	-0.01700	-0.01000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
652	OH-	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
653	OH-	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
654	OH-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
655	OH-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
656	OH-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
657	OH-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
658	OH-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
659	OH-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
660	OH-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
661	OH-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
662	OH-	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
663	OH-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
664	OH-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
665	OH-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
666	HCO3-	CO3=	0.00200	-0.01200	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
667	HCO3-	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
668	HCO3-	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
669	HCO3-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
670	HCO3-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
671	HCO3-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
672	HCO3-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
673	HCO3-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
674	HCO3-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
675	HCO3-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
676	HCO3-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
677	HCO3-	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
678	HCO3-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
679	HCO3-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
680	HCO3-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
681	CO3=	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
682	CO3=	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
683	CO3=	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
684	CO3=	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
685	CO3=	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
686	CO3=	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
687	CO3=	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
688	CO3=	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
689	CO3=	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
690	CO3=	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
691	CO3=	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
692	CO3=	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
693	CO3=	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
694	CO3=	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
695	B(OH)4-	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
696	B(OH)4-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
697	B(OH)4-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
698	B(OH)4-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
699	B(OH)4-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
700	B(OH)4-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
701	B(OH)4-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
702	B(OH)4-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
703	B(OH)4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
704	B(OH)4-	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
705	B(OH)4-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
706	B(OH)4-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
707	B(OH)4-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
708	B3O3(OH)4-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
709	B3O3(OH)4-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
710	B3O3(OH)4-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
711	B3O3(OH)4-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
712	B3O3(OH)4-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
713	B3O3(OH)4-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
714	B3O3(OH)4-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
715	B3O3(OH)4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
716	B3O3(OH)4-	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
717	B3O3(OH)4-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
718	B3O3(OH)4-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
719	B3O3(OH)4-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
720	B4O5(OH)4=	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
721	B4O5(OH)4=	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
722	B4O5(OH)4=	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
723	B4O5(OH)4=	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
724	B4O5(OH)4=	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
725	B4O5(OH)4=	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
726	B4O5(OH)4=	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
727	B4O5(OH)4=	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
728	B4O5(OH)4=	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
729	B4O5(OH)4=	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
730	B4O5(OH)4=	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
731	Br-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
732	Br-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
733	Br-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
734	Br-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

735	Br-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
736	Br-	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
737	Br-	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
738	Br-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
739	Br-	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
740	Br-	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
741	Am(CO3)2-	Am(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
742	Am(CO3)2-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
743	Am(CO3)2-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
744	Am(CO3)2-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
745	Am(CO3)2-	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
746	Am(CO3)2-	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
747	Am(CO3)2-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
748	Am(CO3)2-	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
749	Am(CO3)2-	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
750	Am(CO3)3---	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
751	Am(CO3)3---	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
752	Am(CO3)3---	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
753	Am(CO3)3---	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
754	Am(CO3)3---	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
755	Am(CO3)3---	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
756	Am(CO3)3---	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
757	Am(CO3)3---	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
758	ClO4-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
759	ClO4-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
760	ClO4-	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
761	ClO4-	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
762	ClO4-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
763	ClO4-	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
764	ClO4-	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
765	NpO2(OH)2-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
766	NpO2(OH)2-	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
767	NpO2(OH)2-	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
768	NpO2(OH)2-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
769	NpO2(OH)2-	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
770	NpO2(OH)2-	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
771	NpO2CO3-	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
772	NpO2CO3-	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
773	NpO2CO3-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
774	NpO2CO3-	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
775	NpO2CO3-	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
776	NpO2(CO3)2--	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
777	NpO2(CO3)2--	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
778	NpO2(CO3)2--	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
779	NpO2(CO3)2--	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
780	NpO2(CO3)3---	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
781	NpO2(CO3)3---	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
782	NpO2(CO3)3---	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
783	H2PO4-	HPO4--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
784	H2PO4-	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
785	HPO4--	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
786												
787			Th++++	UO2++	NpO2+							
788	Cl-	SO4--	0.00000	0.00000	0.00000							
789	Cl-	HSO4-	0.00000	0.00000	0.00000							
790	Cl-	OH-	0.00000	0.00000	0.00000							
791	Cl-	HCO3-	0.00000	0.00000	0.00000							
792	Cl-	CO3--	0.00000	0.00000	0.00000							
793	Cl-	B(OH)4-	0.00000	0.00000	0.00000							
794	Cl-	B3O3(OH)4-	0.00000	0.00000	0.00000							
795	Cl-	B4O5(OH)4--	0.00000	0.00000	0.00000							
796	Cl-	Br-	0.00000	0.00000	0.00000							
797	Cl-	Am(CO3)2-	0.00000	0.00000	0.00000							
798	Cl-	Am(CO3)3---	0.00000	0.00000	0.00000							
799	Cl-	ClO4-	0.00000	0.00000	0.00000							
800	Cl-	NpO2(OH)2-	0.00000	0.00000	0.00000							
801	Cl-	NpO2CO3-	0.00000	0.00000	0.00000							
802	Cl-	NpO2(CO3)2--	0.00000	0.00000	0.00000							
803	Cl-	NpO2(CO3)3---	0.00000	0.00000	0.00000							
804	Cl-	H2PO4-	0.00000	0.00000	0.00000							
805	Cl-	HPO4--	0.00000	0.00000	0.00000							
806	Cl-	PO4---	0.00000	0.00000	0.00000							
807	SO4--	HSO4-	0.00000	0.00000	0.00000							
808	SO4--	OH-	0.00000	0.00000	0.00000							
809	SO4--	HCO3-	0.00000	0.00000	0.00000							
810	SO4--	CO3--	0.00000	0.00000	0.00000							
811	SO4--	B(OH)4-	0.00000	0.00000	0.00000							
812	SO4--	B3O3(OH)4-	0.00000	0.00000	0.00000							
813	SO4--	B4O5(OH)4--	0.00000	0.00000	0.00000							
814	SO4--	Br-	0.00000	0.00000	0.00000							
815	SO4--	Am(CO3)2-	0.00000	0.00000	0.00000							
816	SO4--	Am(CO3)3---	0.00000	0.00000	0.00000							
817	SO4--	ClO4-	0.00000	0.00000	0.00000							
818	SO4--	NpO2(OH)2-	0.00000	0.00000	0.00000							
819	SO4--	NpO2CO3-	0.00000	0.00000	0.00000							
820	SO4--	NpO2(CO3)2--	0.00000	0.00000	0.00000							
821	SO4--	NpO2(CO3)3---	0.00000	0.00000	0.00000							
822	SO4--	H2PO4-	0.00000	0.00000	0.00000							
823	SO4--	HPO4--	0.00000	0.00000	0.00000							
824	SO4--	PO4---	0.00000	0.00000	0.00000							
825	HSO4-	OH-	0.00000	0.00000	0.00000							
826	HSO4-	HCO3-	0.00000	0.00000	0.00000							
827	HSO4-	CO3--	0.00000	0.00000	0.00000							
828	HSO4-	B(OH)4-	0.00000	0.00000	0.00000							
829	HSO4-	B3O3(OH)4-	0.00000	0.00000	0.00000							
830	HSO4-	B4O5(OH)4--	0.00000	0.00000	0.00000							
831	HSO4-	Br-	0.00000	0.00000	0.00000							
832	HSO4-	Am(CO3)2-	0.00000	0.00000	0.00000							
833	HSO4-	Am(CO3)3---	0.00000	0.00000	0.00000							
834	HSO4-	ClO4-	0.00000	0.00000	0.00000							
835	HSO4-	NpO2(OH)2-	0.00000	0.00000	0.00000							
836	HSO4-	NpO2CO3-	0.00000	0.00000	0.00000							
837	HSO4-	NpO2(CO3)2--	0.00000	0.00000	0.00000							
838	HSO4-	NpO2(CO3)3---	0.00000	0.00000	0.00000							
839	HSO4-	H2PO4-	0.00000	0.00000	0.00000							
840	HSO4-	HPO4--	0.00000	0.00000	0.00000							
841	HSO4-	PO4---	0.00000	0.00000	0.00000							
842	OH-	HCO3-	0.00000	0.00000	0.00000							
843	OH-	CO3--	0.00000	0.00000	0.00000							
844	OH-	B(OH)4-	0.00000	0.00000	0.00000							
845	OH-	B3O3(OH)4-	0.00000	0.00000	0.00000							
846	OH-	B4O5(OH)4--	0.00000	0.00000	0.00000							
847	OH-	Br-	0.00000	0.00000	0.00000							
848	OH-	Am(CO3)2-	0.00000	0.00000	0.00000							
849	OH-	Am(CO3)3---	0.00000	0.00000	0.00000							
850	OH-	ClO4-	0.00000	0.00000	0.00000							
851	OH-	NpO2(OH)2-	0.00000	0.00000	0.00000							
852	OH-	NpO2CO3-	0.00000	0.00000	0.00000							
853	OH-	NpO2(CO3)2--	0.00000	0.00000	0.00000							
854	OH-	NpO2(CO3)3---	0.00000	0.00000	0.00000							
855	OH-	H2PO4-	0.00000	0.00000	0.00000							
856	OH-	HPO4--	0.00000	0.00000	0.00000							
857	OH-	PO4---	0.00000	0.00000	0.00000							
858	HCO3-	CO3--	0.00000	0.00000	0.00000							

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

859	HCO3-	B(OH)4-	0.00000	0.00000	0.00000
860	HCO3-	B3O3(OH)4-	0.00000	0.00000	0.00000
861	HCO3-	B4O5(OH)4=	0.00000	0.00000	0.00000
862	HCO3-	Br-	0.00000	0.00000	0.00000
863	HCO3-	Am(CO3)2-	0.00000	0.00000	0.00000
864	HCO3-	Am(CO3)3=-	0.00000	0.00000	0.00000
865	HCO3-	ClO4-	0.00000	0.00000	0.00000
866	HCO3-	NpO2(OH)2-	0.00000	0.00000	0.00000
867	HCO3-	NpO2CO3-	0.00000	0.00000	0.00000
868	HCO3-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
869	HCO3-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
870	HCO3-	H2PO4-	0.00000	0.00000	0.00000
871	HCO3-	HPO4=	0.00000	0.00000	0.00000
872	HCO3-	PO4=-	0.00000	0.00000	0.00000
873	CO3=	B(OH)4-	0.00000	0.00000	0.00000
874	CO3=	B3O3(OH)4-	0.00000	0.00000	0.00000
875	CO3=	B4O5(OH)4=	0.00000	0.00000	0.00000
876	CO3=	Br-	0.00000	0.00000	0.00000
877	CO3=	Am(CO3)2-	0.00000	0.00000	0.00000
878	CO3=	Am(CO3)3=-	0.00000	0.00000	0.00000
879	CO3=	ClO4-	0.00000	0.00000	0.00000
880	CO3=	NpO2(OH)2-	0.00000	0.00000	0.00000
881	CO3=	NpO2CO3-	0.00000	0.00000	0.00000
882	CO3=	NpO2(CO3)2=-	0.00000	0.00000	0.00000
883	CO3=	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
884	CO3=	H2PO4-	0.00000	0.00000	0.00000
885	CO3=	HPO4=	0.00000	0.00000	0.00000
886	CO3=	PO4=-	0.00000	0.00000	0.00000
887	B(OH)4-	B3O3(OH)4-	0.00000	0.00000	0.00000
888	B(OH)4-	B4O5(OH)4=	0.00000	0.00000	0.00000
889	B(OH)4-	Br-	0.00000	0.00000	0.00000
890	B(OH)4-	Am(CO3)2-	0.00000	0.00000	0.00000
891	B(OH)4-	Am(CO3)3=-	0.00000	0.00000	0.00000
892	B(OH)4-	ClO4-	0.00000	0.00000	0.00000
893	B(OH)4-	NpO2(OH)2-	0.00000	0.00000	0.00000
894	B(OH)4-	NpO2CO3-	0.00000	0.00000	0.00000
895	B(OH)4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
896	B(OH)4-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
897	B(OH)4-	H2PO4-	0.00000	0.00000	0.00000
898	B(OH)4-	HPO4=	0.00000	0.00000	0.00000
899	B(OH)4-	PO4=-	0.00000	0.00000	0.00000
900	B3O3(OH)4-	B4O5(OH)4=	0.00000	0.00000	0.00000
901	B3O3(OH)4-	Br-	0.00000	0.00000	0.00000
902	B3O3(OH)4-	Am(CO3)2-	0.00000	0.00000	0.00000
903	B3O3(OH)4-	Am(CO3)3=-	0.00000	0.00000	0.00000
904	B3O3(OH)4-	ClO4-	0.00000	0.00000	0.00000
905	B3O3(OH)4-	NpO2(OH)2-	0.00000	0.00000	0.00000
906	B3O3(OH)4-	NpO2CO3-	0.00000	0.00000	0.00000
907	B3O3(OH)4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
908	B3O3(OH)4-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
909	B3O3(OH)4-	H2PO4-	0.00000	0.00000	0.00000
910	B3O3(OH)4-	HPO4=	0.00000	0.00000	0.00000
911	B3O3(OH)4-	PO4=-	0.00000	0.00000	0.00000
912	B4O5(OH)4=	Br-	0.00000	0.00000	0.00000
913	B4O5(OH)4=	Am(CO3)2-	0.00000	0.00000	0.00000
914	B4O5(OH)4=	Am(CO3)3=-	0.00000	0.00000	0.00000
915	B4O5(OH)4=	ClO4-	0.00000	0.00000	0.00000
916	B4O5(OH)4=	NpO2(OH)2-	0.00000	0.00000	0.00000
917	B4O5(OH)4=	NpO2CO3-	0.00000	0.00000	0.00000
918	B4O5(OH)4=	NpO2(CO3)2=-	0.00000	0.00000	0.00000
919	B4O5(OH)4=	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
920	B4O5(OH)4=	H2PO4-	0.00000	0.00000	0.00000
921	B4O5(OH)4=	HPO4=	0.00000	0.00000	0.00000
922	B4O5(OH)4=	PO4=-	0.00000	0.00000	0.00000
923	Br-	Am(CO3)2-	0.00000	0.00000	0.00000
924	Br-	Am(CO3)3=-	0.00000	0.00000	0.00000
925	Br-	ClO4-	0.00000	0.00000	0.00000
926	Br-	NpO2(OH)2-	0.00000	0.00000	0.00000
927	Br-	NpO2CO3-	0.00000	0.00000	0.00000
928	Br-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
929	Br-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
930	Br-	H2PO4-	0.00000	0.00000	0.00000
931	Br-	HPO4=	0.00000	0.00000	0.00000
932	Br-	PO4=-	0.00000	0.00000	0.00000
933	Am(CO3)2-	Am(CO3)3=-	0.00000	0.00000	0.00000
934	Am(CO3)2-	ClO4-	0.00000	0.00000	0.00000
935	Am(CO3)2-	NpO2(OH)2-	0.00000	0.00000	0.00000
936	Am(CO3)2-	NpO2CO3-	0.00000	0.00000	0.00000
937	Am(CO3)2-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
938	Am(CO3)2-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
939	Am(CO3)2-	H2PO4-	0.00000	0.00000	0.00000
940	Am(CO3)2-	HPO4=	0.00000	0.00000	0.00000
941	Am(CO3)2-	PO4=-	0.00000	0.00000	0.00000
942	Am(CO3)3=-	ClO4-	0.00000	0.00000	0.00000
943	Am(CO3)3=-	NpO2(OH)2-	0.00000	0.00000	0.00000
944	Am(CO3)3=-	NpO2CO3-	0.00000	0.00000	0.00000
945	Am(CO3)3=-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
946	Am(CO3)3=-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
947	Am(CO3)3=-	H2PO4-	0.00000	0.00000	0.00000
948	Am(CO3)3=-	HPO4=	0.00000	0.00000	0.00000
949	Am(CO3)3=-	PO4=-	0.00000	0.00000	0.00000
950	ClO4-	NpO2(OH)2-	0.00000	0.00000	0.00000
951	ClO4-	NpO2CO3-	0.00000	0.00000	0.00000
952	ClO4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
953	ClO4-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
954	ClO4-	H2PO4-	0.00000	0.00000	0.00000
955	ClO4-	HPO4=	0.00000	0.00000	0.00000
956	ClO4-	PO4=-	0.00000	0.00000	0.00000
957	NpO2(OH)2-	NpO2CO3-	0.00000	0.00000	0.00000
958	NpO2(OH)2-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
959	NpO2(OH)2-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
960	NpO2(OH)2-	H2PO4-	0.00000	0.00000	0.00000
961	NpO2(OH)2-	HPO4=	0.00000	0.00000	0.00000
962	NpO2(OH)2-	PO4=-	0.00000	0.00000	0.00000
963	NpO2CO3-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
964	NpO2CO3-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
965	NpO2CO3-	H2PO4-	0.00000	0.00000	0.00000
966	NpO2CO3-	HPO4=	0.00000	0.00000	0.00000
967	NpO2CO3-	PO4=-	0.00000	0.00000	0.00000
968	NpO2(CO3)2=-	NpO2(CO3)3=4-	0.00000	0.00000	0.00000
969	NpO2(CO3)2=-	H2PO4-	0.00000	0.00000	0.00000
970	NpO2(CO3)2=-	HPO4=	0.00000	0.00000	0.00000
971	NpO2(CO3)2=-	PO4=-	0.00000	0.00000	0.00000
972	NpO2(CO3)3=4-	H2PO4-	0.00000	0.00000	0.00000
973	NpO2(CO3)3=4-	HPO4=	0.00000	0.00000	0.00000
974	NpO2(CO3)3=4-	PO4=-	0.00000	0.00000	0.00000
975	H2PO4-	HPO4=	0.00000	0.00000	0.00000
976	H2PO4-	PO4=-	0.00000	0.00000	0.00000
977	HPO4=	PO4=-	0.00000	0.00000	0.00000
978					

979 Neutral-Cation Binary Interactions: lambda(n,c)

980

981		CO2(aq)	CaCO3(aq)	MgCO3(aq)	B(OH)3(aq)	NpO2OH(aq)	H3PO4(aq)
982	Na+	0.10000	0.00000	0.00000	-0.09700	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

983	K+	0.05100	0.00000	0.00000	-0.14000	0.00000	-0.07000
984	Ca++	0.18300	0.00000	0.00000	0.00000	0.00000	0.00000
985	Mg++	0.18300	0.00000	0.00000	0.00000	0.00000	0.00000
986	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
987	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.29000
988	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
989	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
990	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
991	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
992	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
993	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
994	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
995							
996							
997	Neutral- Anion Binary Interactions: lambda(n,a)						
998							
999		CO2(aq)	CaCO3(aq)	MgCO3(aq)	B(OH)3(aq)	NpO2OH(aq)	H3PO4(aq)
1000	Cl-	-0.00500	0.00000	0.00000	0.09100	0.00000	0.00000
1001	SO4=	0.09700	0.00000	0.00000	0.01800	0.00000	0.00000
1002	HSO4-	-0.00300	0.00000	0.00000	0.00000	0.00000	0.00000
1003	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1004	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1005	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1006	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1007	B3O3(OH)4-	0.00000	0.00000	0.00000	-0.20000	0.00000	0.00000
1008	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1009	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1010	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1011	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1012	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1013	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1014	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1015	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1016	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1017	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	-0.40000
1018	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1019	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1020							
1021	Neutral-Cation-Anion Ternary Interactions: zeta(n,c,a)						
1022							
1023							
1024			CO2(aq)	CaCO3(aq)	MgCO3(aq)	B(OH)3(aq	NpO2OH(aq	H3PO4(aq)
1025	Na+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1026	Na+	SO4=	0.00000	0.00000	0.00000	0.04600	0.00000	0.00000
1027	Na+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1028	Na+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1029	Na+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1030	Na+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1031	Na+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1032	Na+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1033	Na+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1034	Na+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1035	Na+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1036	Na+	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1037	Na+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1038	Na+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1039	Na+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1040	Na+	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1041	Na+	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1042	Na+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1043	Na+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1044	Na+	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1045	K+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1046	K+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1047	K+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1048	K+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1049	K+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1050	K+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1051	K+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1052	K+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1053	K+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1054	K+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1055	K+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1056	K+	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1057	K+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1058	K+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1059	K+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1060	K+	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1061	K+	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1062	K+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1063	K+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1064	K+	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1065	Ca++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1066	Ca++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1067	Ca++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1068	Ca++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1069	Ca++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1070	Ca++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1071	Ca++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1072	Ca++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1073	Ca++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1074	Ca++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1075	Ca++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1076	Ca++	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1077	Ca++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1078	Ca++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1079	Ca++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1080	Ca++	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1081	Ca++	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1082	Ca++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1083	Ca++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1084	Ca++	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1085	Mg++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1086	Mg++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1087	Mg++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1088	Mg++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1089	Mg++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1090	Mg++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1091	Mg++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1092	Mg++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1093	Mg++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1094	Mg++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1095	Mg++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1096	Mg++	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1097	Mg++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1098	Mg++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1099	Mg++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1100	Mg++	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1101	Mg++	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1102	Mg++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1103	Mg++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1104	Mg++	PO4---	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1105	MgOH+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1106	MgOH+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

1107	MgOH+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1108	MgOH+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1109	MgOH+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1110	MgOH+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1111	MgOH+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1112	MgOH+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1113	MgOH+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1114	MgOH+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1115	MgOH+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1116	MgOH+	Am(CO3)3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1117	MgOH+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1118	MgOH+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1119	MgOH+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1120	MgOH+	NpO2(CO3)2=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1121	MgOH+	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1122	MgOH+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1123	MgOH+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1124	MgOH+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1125	H+	Cl-	0.00000	0.00000	0.00000	-0.01020	0.00000	0.00000
1126	H+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1127	H+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1128	H+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1129	H+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1130	H+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1131	H+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1132	H+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1133	H+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1134	H+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1135	H+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1136	H+	Am(CO3)3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1137	H+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1138	H+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1139	H+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1140	H+	NpO2(CO3)2=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1141	H+	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1142	H+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1143	H+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1144	H+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1145	MgB(OH)4+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1146	MgB(OH)4+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1147	MgB(OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1148	MgB(OH)4+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1149	MgB(OH)4+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1150	MgB(OH)4+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1151	MgB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1152	MgB(OH)4+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1153	MgB(OH)4+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1154	MgB(OH)4+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1155	MgB(OH)4+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1156	MgB(OH)4+	Am(CO3)3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1157	MgB(OH)4+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1158	MgB(OH)4+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1159	MgB(OH)4+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1160	MgB(OH)4+	NpO2(CO3)2=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1161	MgB(OH)4+	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1162	MgB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1163	MgB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1164	MgB(OH)4+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1165	CaB(OH)4+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1166	CaB(OH)4+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1167	CaB(OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1168	CaB(OH)4+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1169	CaB(OH)4+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1170	CaB(OH)4+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1171	CaB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1172	CaB(OH)4+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1173	CaB(OH)4+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1174	CaB(OH)4+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1175	CaB(OH)4+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1176	CaB(OH)4+	Am(CO3)3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1177	CaB(OH)4+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1178	CaB(OH)4+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1179	CaB(OH)4+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1180	CaB(OH)4+	NpO2(CO3)2=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1181	CaB(OH)4+	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1182	CaB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1183	CaB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1184	CaB(OH)4+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1185	Am+++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1186	Am+++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1187	Am+++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1188	Am+++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1189	Am+++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1190	Am+++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1191	Am+++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1192	Am+++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1193	Am+++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1194	Am+++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1195	Am+++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1196	Am+++	Am(CO3)3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1197	Am+++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1198	Am+++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1199	Am+++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1200	Am+++	NpO2(CO3)2=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1201	Am+++	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1202	Am+++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1203	Am+++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1204	Am+++	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1205	AmCO3+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1206	AmCO3+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1207	AmCO3+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1208	AmCO3+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1209	AmCO3+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1210	AmCO3+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1211	AmCO3+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1212	AmCO3+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1213	AmCO3+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1214	AmCO3+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1215	AmCO3+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1216	AmCO3+	Am(CO3)3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1217	AmCO3+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1218	AmCO3+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1219	AmCO3+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1220	AmCO3+	NpO2(CO3)2=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1221	AmCO3+	NpO2(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1222	AmCO3+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1223	AmCO3+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1224	AmCO3+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1225	Th++++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1226	Th++++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1227	Th++++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1228	Th++++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1229	Th++++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1230	Th++++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

```
1231  Th++++          B(OH)4-          0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1232  Th++++          B3O3(OH)4-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1233  Th++++          B4O5(OH)4=       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1234  Th++++          Br-              0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1235  Th++++          Am(CO3)2-        0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1236  Th++++          Am(CO3)3=-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1237  Th++++          ClO4-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1238  Th++++          NpO2(OH)2-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1239  Th++++          NpO2CO3-         0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1240  Th++++          NpO2(CO3)2=-     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1241  Th++++          NpO2(CO3)3=5-    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1242  Th++++          H2PO4-           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1243  Th++++          HPO4=            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1244  Th++++          PO4=-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1245  UO2++           Cl-              0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1246  UO2++           SO4=             0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1247  UO2++           HSO4-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1248  UO2++           OH-              0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1249  UO2++           HCO3-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1250  UO2++           CO3=             0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1251  UO2++           B(OH)4-          0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1252  UO2++           B3O3(OH)4-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1253  UO2++           B4O5(OH)4=       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1254  UO2++           Br-              0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1255  UO2++           Am(CO3)2-        0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1256  UO2++           Am(CO3)3=-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1257  UO2++           ClO4-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1258  UO2++           NpO2(OH)2-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1259  UO2++           NpO2CO3-         0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1260  UO2++           NpO2(CO3)2=-     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1261  UO2++           NpO2(CO3)3=5-    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1262  UO2++           H2PO4-           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1263  UO2++           HPO4=            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1264  UO2++           PO4=-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1265  NpO2+           Cl-              0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1266  NpO2+           SO4=             0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1267  NpO2+           HSO4-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1268  NpO2+           OH-              0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1269  NpO2+           HCO3-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1270  NpO2+           CO3=             0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1271  NpO2+           B(OH)4-          0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1272  NpO2+           B3O3(OH)4-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1273  NpO2+           B4O5(OH)4=       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1274  NpO2+           Br-              0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1275  NpO2+           Am(CO3)2-        0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1276  NpO2+           Am(CO3)3=-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1277  NpO2+           ClO4-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1278  NpO2+           NpO2(OH)2-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1279  NpO2+           NpO2CO3-         0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1280  NpO2+           NpO2(CO3)2=-     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1281  NpO2+           NpO2(CO3)3=5-    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1282  NpO2+           H2PO4-           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1283  NpO2+           HPO4=            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1284  NpO2+           PO4=-            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
1285  using PITZER ACTIVITY COEFFICIENT model
1286  Charge Balance replaces element Oxygen
1287
1288
1289  this is a BATCH problem
1290
1291  FOR088    file name is U1:[SCBABB.FMT.UM]BATCH_DOC.FOR088;1
1292
1293  Ideal Gas Constant is Unity (Dimensionless)
1294  Temperature =       298.15 [=] degree Kelvin
1295
1296
1297    115 Species                        23 Elements
1298
1299          Element Name          Molecular Weight
1300          Hydrogen                      1.00790
1301          Oxygen                       15.99940
1302          Sodium                       22.98977
1303          Potassium                    39.09830
1304          Magnesium                    24.30500
1305          Calcium                      40.08000
1306          Chlorine                     35.45300
1307          Sulfur                       32.06000
1308          Carbon                       12.01100
1309          PosIon                        0.00000
1310          NegIon                        0.00000
1311          Air                          28.84000
1312          Boron                        10.81000
1313          Bromine                      79.90400
1314          TracerEl                      0.00000
1315          Th(IV)                      232.03810
1316          Am(III)                     243.00000
1317          U(VI)                       238.02900
1318          Np(V)                       237.04820
1319          ClO4-(EL)                    99.45060
1320          Phosphorus                   30.97400
1321          Electron                      0.00000
1322          Charge                        0.00000
1323
1324
1325      Species Name                              Phase        Mol.Wt.    Std Chemical Potential, u/RT
1326    1 H2O                                WATER  aqueous      18.015      -95.6635
1327    2 Na+                                 Na+   aqueous      22.990     -105.6510
1328    3 K+                                  K+    aqueous      39.098     -113.9570
1329    4 Ca++                               Ca++   aqueous      40.080     -223.3000
1330    5 Mg++                               Mg++   aqueous      24.305     -183.4680
1331    6 MgOH+                             MgOH+   aqueous      41.312     -251.9400
1332    7 H+                                  H+    aqueous       1.008        0.0000
1333    8 Cl-                                 Cl-   aqueous      35.453      -52.9550
1334    9 SO4=                               SO4=   aqueous      96.058     -300.3860
1335   10 HSO4-                             HSO4-   aqueous      97.066     -304.9620
1336   11 OH-                                OH-    aqueous      17.007      -63.4350
1337   12 HCO3-                             HCO3-   aqueous      61.017     -236.7510
1338   13 CO3=                               CO3=   aqueous      60.009     -212.9440
1339   14 CO2(aq)                         CO2(aq)   aqueous      44.010     -155.6800
1340   15 CaCO3(aq)                     CaCO3(aq)   aqueous     100.089     -443.5000
1341   16 MgCO3(aq)                     MgCO3(aq)   aqueous      84.314     -403.1550
1342   17 B(OH)3(aq)                    B(OH)3(aq)  aqueous      61.832     -390.8100
1343   18 B(OH)4-                        B(OH)4-    aqueous      78.839     -465.2000
1344   19 B3O3(OH)4-                    B3O3(OH)4-  aqueous     148.457     -963.7700
1345   20 B4O5(OH)4=                    B4O5(OH)4=  aqueous     191.266    -1239.1000
1346   21 CaB(OH)4+                      CaB(OH)4+  aqueous     118.919     -692.3000
1347   22 MgB(OH)4+                      MgB(OH)4+  aqueous     103.144     -651.8900
1348   23 Br-                                Br-    aqueous      79.904     -999.9900
1349   24 ClO4-                 perchlorate ClO4-   aqueous      99.451     -999.9900
1350   25 NaOH(aq).....to.titrate.base.only         aqueous      39.997      500.0000
1351   26 HCl(aq).....to.titrate.acid.only          aqueous      36.461      500.0000
1352   27 HClO4(aq).....to.titrate.acid.only        aqueous     100.459      500.0000
1353   28 PosIon.................POSITIVE.ION       aqueous       0.000        0.0000
1354   29 NegIon.................NEGATIVE.ION       aqueous       0.000        0.0000
```

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

30	PosIon(OH)(aq).....	to.titrate.base	aqueous	17.007	500.0000	
31	HNegIon(aq).....	to.titrate.acid	aqueous	1.008	500.0000	
32	Tracer(aq).....	conservative.tracer	aqueous	0.000	0.0000	
33	H3PO4(aq)	H3PO4(aq)	aqueous	97.995	-460.9000	
34	H2PO4-	H2PO4-	aqueous	96.987	-455.9600	
35	HPO4=	HPO4=	aqueous	95.980	-439.3670	
36	PO4=-	PO4=-	aqueous	94.972	-410.9470	
37	NpO2+	NpO2+	aqueous	269.047	-369.1270	
38	NpO2OH(aq)	NpO2OH(aq)	aqueous	286.054	-438.5180	
39	NpO2(OH)2-	NpO2(OH)2-	aqueous	303.062	-505.8290	
40	NpO2CO3-	NpO2CO3-	aqueous	329.056	-594.4920	
41	NpO2(CO3)2=-	NpO2(CO3)2=-	aqueous	389.065	-808.4030	
42	NpO2(CO3)3===	NpO2(CO3)3===	aqueous	449.075	-1019.9180	
43	Am+++	Am+++	aqueous	243.000	-241.6940	
44	AmCO3+	AmCO3+	aqueous	303.009	-472.0600	
45	Am(CO3)2-	Am(CO3)2-	aqueous	363.018	-695.8800	
46	Am(CO3)3=-	Am(CO3)3=-	aqueous	423.028	-915.4600	
47	Am(OH)2+	Am(OH)2+	aqueous	277.015	-393.6470	
48	Am(OH)3(aq)	Am(OH)3(aq)	aqueous	294.022	-462.9500	
49	Th++++	Th++++	aqueous	232.038	-999.9900	
50	UO2++	U(VI)O2++	aqueous	270.028	-999.9900	
51	NpO2OH(aged)_____	NpO2OH(aged)	solid	286.054	-454.0100	
52	NpO2OH(amor)_____	NpO2OH(amor)	solid	286.054	-452.6420	
53	NaNpO2CO3(s)_____	NaNpO2CO3(s)	solid	352.046	-713.7070	
54	Na3NpO2(CO3)2(s)_DISABLED_DISABLED		solid	458.035	999.9900	
55	AmOHCO3(c)_____	AmOHCO3(c)	solid	320.017	-569.9800	
56	Am(OH)3(s)_____	Am(OH)3(s)	solid	294.022	-492.2940	
57	NaAm(CO3)2.6H2O(c)_____		solid	494.099	-1396.4940	
58	AmPO4(c)_____	AmPO4(c)	solid	337.972	-709.7500	
59	CaSO4_____	Anhydrite	solid	136.138	-533.7300	
60	NaK3(SO4)2__	Aphthitalite/Glaserite	solid	332.400	-1057.0500	
61	CaCl2.6H2O_____	Antarcticite	solid	219.077	-893.6500	
62	CaCO3_____	Aragonite	solid	100.089	-455.1700	
63	K2SO4_____	Arcanite	solid	174.254	-532.3900	
64	MgCl2.6H2O_____	Bischofite	solid	203.302	-853.1000	
65	Na2Mg(SO4)2.4H2O_____	Bloedite	solid	334.461	-1383.6000	
66	Mg(OH)2_____	Brucite	solid	58.320	-335.4000	
67	Na6CO3(SO4)2_____	Burkeite	solid	390.063	-1449.4000	
68	CaCO3_____	Calcite	solid	100.089	-455.6000	
69	CaCl2.4H2O_____	CaCl2_Tetrahydrite	solid	183.047	-698.7000	
70	Ca4Cl2(OH)6.13H2O__	CaOxychloride A	solid	567.467	-2658.4500	
71	Ca2Cl2(OH)2.H2O____	CaOxychloride B	solid	203.096	-778.4100	
72	KMgCl3.6H2O_____	Carnallite	solid	277.854	-1020.3000	
73	MgSO4.7H2O_____	Epsomite	solid	246.469	-1157.8300	
74	CaNa2(CO3)2.5H2O_____	Gaylussite	solid	296.154	-1360.5000	
75	Na2Ca(SO4)2_____	Glauberite	solid	278.175	-1047.4500	
76	CaSO4.2H2O_____	Gypsum	solid	172.168	-725.5600	
77	NaCl_____	Halite	solid	58.443	-154.9900	
78	MgSO4.6H2O_____	Hexahydrite	solid	228.454	-1061.6000	
79	KMgClSO4.3H2O_____	Kainite	solid	248.960	-938.2000	
80	KHCO3_____	Kalicinite	solid	100.115	-350.0600	
81	MgSO4.H2O_____	Kieserite	solid	138.378	-579.8000	
82	K2Mg(SO4)2.4H2O_____	Leonite	solid	366.678	-1403.9700	
83	Na4Ca(SO4)3.2H2O_____	Labile_Salt	solid	456.242	-1751.4500	
84	MgCO3_____	Magnesite	solid	84.314	-414.4500	
85	Mg2Cl(OH)3.4H2O_____	MgOxychloride	solid	207.146	-1029.6000	
86	KHSO4_____	Mercallite	solid	136.164	-617.5700	
87	Na2SO4.10H2O_____	Mirabilite	solid	322.189	-1471.1500	
88	K6H6(SO4)7_____	Niesnite	solid	991.237	-3039.2400	
89	NaHCO3_____	Nahcolite	solid	84.007	-343.3300	
90	Na2CO3.10H2O_____	Natron	solid	286.141	-1382.7800	
91	MgCO3.3H2O_____	Nesquehonite	solid	138.360	-695.3000	
92	K2Mg(SO4)2.6H2O Picromerite/Schoen		solid	402.708	-1596.1000	
93	Na2Ca(CO3)2.2H2O_____	Pirssonite	solid	242.108	-1073.1000	
94	K2MgCa2(SO4)4.2H2O_____	Polyhalite	solid	602.922	-2262.5000	
95	Ca(OH)2_____	Portlandite	solid	74.095	-362.1200	
96	K2CO3.3/2H2O___	Potassium_Carbonate	solid	165.229	-577.3700	
97	K8H4(CO3)6.3H2O___	K-Sequicarbonate	solid	730.919	-2555.4000	
98	KNaCO3.6H2O_____	K-Na-Carbonate	solid	230.188	-1006.8000	
99	K2NaH(CO3)2.2H2O___	Potassium_Trona	solid	258.243	-971.7400	
100	K3H(SO4)2__	Sesquipotassium_Sulfate	solid	310.418	-950.8000	
101	Na3H(SO4)2____	Sesquisodium_Sulfate	solid	262.092	-919.6000	
102	Na2CO3.7H2O____	Na2CO3-Heptahydrate	solid	232.095	-1094.9500	
103	KCl_____	Sylvite	solid	74.551	-164.8400	
104	K2Ca(SO4)2.H2O_____	Syngenite	solid	328.407	-1164.8000	
105	Mg2CaCl6.12H2O_____	Tachyhydrite	solid	517.590	-2015.9000	
106	Na2SO4_____	Thenardite	solid	142.037	-512.3500	
107	Na2CO3.H2O_____	Thermonatrite	solid	124.004	-518.8000	
108	Na3H(CO3)2.2H2O_____	Trona	solid	226.026	-960.3800	
109	Na2B4O7.10H2O_____	Borax	solid	381.367	-2224.1600	
110	B(OH)3_____	Borix_Acid_Solid	solid	61.832	-390.8800	
111	KB5O8.4H2O____	K-Pentaborate_(30_C)	solid	293.204	-1770.2600	
112	K2B4O7.4H2O___	K-Tetraborate_(30_C)	solid	305.493	-1663.4700	
113	NaBO2.4H2O_____	Sodium_Metaborate	solid	137.859	-761.4200	
114	NaB5O8.5H2O____	Sodium_Pentaborate	solid	295.111	-1854.8000	
115	NaBO2.NaCl.2H2O___	Teepleite_(20_C)	solid	160.272	-725.7700	

Truncated Name — Formula Matrix

1	H2O	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	Na+	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
3	K+	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
4	Ca++	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
5	Mg++	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
6	MgOH+	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
7	H+	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
8	Cl-	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
9	SO4=	0	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2
10	HSO4-	1	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
11	OH-	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
12	HCO3-	1	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
13	CO3=	0	3	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2
14	CO2(aq)	0	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	CaCO3(aq)	0	3	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	MgCO3(aq)	0	3	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	B(OH)3(aq)	3	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
18	B(OH)4-	4	4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
19	B3O3(OH)4-	4	7	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	-1
20	B4O5(OH)4=	4	9	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	-2
21	CaB(OH)4+	4	4	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
22	MgB(OH)4+	4	4	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
23	Br-	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-1
24	ClO4- pe	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	NaOH(aq).....to.ti	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-1
26	HCl(aq).....to.ti	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	HClO4(aq).....to.ti	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
28	PosIon.....	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1
29	NegIon.....	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	-1
30	PosIon(OH)(aq).....	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	HNegIon(aq).....	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
32	Tracer(aq).....cons	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
33	H3PO4(aq)	3	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
34	H2PO4-	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-1
35	HPO4=	1	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-2

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

```
1479   36 PO4+-                    0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0 -1
1480   37 NpO2+                    0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  1
1481   38 NpO2OH(aq)               1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0
1482   39 NpO2(OH)2-               2  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0 -1
1483   40 NpO2CO3-                 0  5  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  1  0  0  0 -1
1484   41 NpO2(CO3)2=-             0  8  0  0  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  1  0  0  0 -3
1485   42 NpO2(CO3)3---            0 11  0  0  0  0  0  0  0  3  0  0  0  0  0  0  0  0  0  1  0  0  0 -5
1486   43 Am+++                    0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  3
1487   44 AmCO3+                   0  3  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  1  0  0  0  0  0  1
1488   45 Am(CO3)2-                0  6  0  0  0  0  0  0  0  2  0  0  0  0  0  0  0  1  0  0  0  0  0 -1
1489   46 Am(CO3)3=-               0  9  0  0  0  0  0  0  0  3  0  0  0  0  0  0  0  1  0  0  0  0  0 -3
1490   47 Am(OH)2+                 2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  1
1491   48 Am(OH)3(aq)              3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0
1492   49 Tb++++                   0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  4
1493   50 UO2++                    0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  2
1494   51 NpO2OH(aged)_____        1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0
1495   52 NpO2OH(amor)_____        1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0
1496   53 NaNpO2CO3(s)_____        0  5  1  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  1  0  0  0  0
1497   54 Na3NpO2(CO3)2(s)_DI      0  8  3  0  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  1  0  0  0  0
1498   55 AmOHCO3(c)_____          1  4  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  1  0  0  0  0  0  0
1499   56 Am(OH)3(s)_____          3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0
1500   57 NaAm(CO3)2.6H2O(c)_      12 12  1  0  0  0  0  0  0  2  0  0  0  0  0  0  0  1  0  0  0  0  0  0
1501   58 AmPO4(c)_____            0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  1  0  0
1502   59 CaSO4_____               0  4  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1503   60 NaKJ(SO4)2__Aphthit      0  8  1  3  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1504   61 CaCl2.6H2O_____          12  6  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1505   62 CaCO3_____               0  3  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1506   63 K2SO4_____               0  4  0  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1507   64 MgCl2.6H2O_____          12  6  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1508   65 Na2Mg(SO4)2.4H2O___      8 12  2  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1509   66 Mg(OH)2_____             2  2  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1510   67 Na6CO3(SO4)2_____        0 11  6  0  0  0  0  2  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1511   68 CaCO3_____               0  3  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1512   69 CaCl2.4H2O_____CaC       8  4  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1513   70 Ca4Cl2(OH)6.13H2O__      32 19  0  0  0  4  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1514   71 Ca2Cl2(OH)2.H2O____      4  3  0  0  0  2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1515   72 KMgCl3.6H2O_____         12  6  0  1  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1516   73 MgSO4.7H2O_____          14 11  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1517   74 CaNa2(CO3)2.5H2O___      10 11  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1518   75 Na2Ca(SO4)2_____         0  8  2  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1519   76 CaSO4.2H2O_____          4  6  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1520   77 NaCl_____                0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1521   78 MgSO4.6H2O_____          12 10  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1522   79 KMgClSO4.3H2O_____       6  7  0  1  1  0  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1523   80 KHCO3_____               1  3  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1524   81 MgSO4.H2O_____           2  5  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1525   82 K2Mg(SO4)2.4H2O___       8 12  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1526   83 Na4Ca(SO4)3.2H2O___      4 14  4  0  0  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1527   84 MgCO3_____               0  3  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1528   85 Mg2Cl(OH)3.4H2O____      11  7  0  0  2  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1529   86 KHSO4_____               1  4  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1530   87 Na2SO4.10H2O_____        20 14  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1531   88 K8H6(SO4)7_____          6 28  0  8  0  0  0  7  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1532   89 NaHCO3_____              1  3  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1533   90 Na2CO3.10H2O_____        20 13  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1534   91 MgCO3.3H2O_____          6  6  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1535   92 K2Mg(SO4)2.6H2O Pic      12 14  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1536   93 Na2Ca(CO3)2.2H2O___      4  8  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1537   94 K2MgCa2(SO4)4.2H2O_      4 18  0  2  1  2  0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1538   95 Ca(OH)2_____             2  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1539   96 K2CO3.3/2H2O___Pota      3  4  0  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1540   97 K8H4(CO3)6.3H2O___K      10 21  0  8  0  0  0  0  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1541   98 KNaCO3.6H2O_____         12  9  1  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1542   99 K2NaH(CO3)2.2H2O___      5  8  1  2  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1543  100 KJH(SO4)2__Sesquipo      1  8  0  3  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1544  101 NaJH(SO4)2____Sesqu      1  8  3  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1545  102 Na2CO3.7H2O____Na2C      14 10  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1546  103 KCl_____                0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1547  104 K2Ca(SO4)2.H2O_____     2  9  0  2  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1548  105 Mg2CaCl6.12H2O_____     24 12  0  0  2  1  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1549  106 Na2SO4_____             0  4  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1550  107 Na2CO3.H2O_____         2  4  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1551  108 Na3H(CO3)2.2H2O____     5  8  3  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1552  109 Na2B4O7.10H2O_____      20 17  2  0  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0  0
1553  110 B(OH)3_____B            3  3  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
1554  111 KB5O8.4H2O____K-Pen     8 12  0  1  0  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0  0
1555  112 K2B4O7.4H2O___K-Tet     8 11  0  2  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0  0
1556  113 NaBO2.4H2O_____So       8  6  1  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
1557  114 NaBSO8.5H2O____Sod      10 13  1  0  0  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0  0
1558  115 NaBO2.NaCl.2H2O___T     4  4  2  0  0  0  1  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
1559  ************************************************************************************************************
1560
```

Appendix K: Listing of HMW_NP_AM_RTEST.RHOMIN and References Cited in Listing

K.1 Listing

See Table 12 for explanation of this listing.

```
1       2.d3    'Np(V)O2OH(aged)....Np(V)O2OH(aged)'
2       2.d3    'Np(V)O2OH(amor)....Np(V)O2OH(amor)'
3       2.d3    'NaNp(V)O2CO3(s)....NaNp(V)O2CO3(s)'
4       2.d3    'NaNpO2CO3Na2CO3(s)Na3NpO2(CO3)2(s)'
5       2.d3    AmOHCO3(c)
6       2.d3    Am(OH)3(s)
7       2.d3    NaAm(CO3)2.6H2O(c)
8       2.d3    'AmPO4(c)
9
10   2980.d0    CaSO4                       Anhydrite  CRC p.B-181:185
11      2.d3    NaKJ(SO4)2  Aphthitalite/Glaserite
12      2.d3    CaCl2.6H2O                Antarcticite
13   2940.d0    CaCO3                       Aragonite  CRC p.B-181:185
14   2663.d0    K2SO4                       Arcanite   CRC p.B-181:185
15      2.d3    MgCl2.6H2O                Bischofite
16   2250.d0    Na2Mg(SO4)2.4H2O            Bloedite   CRC p.B-181:185
17   2390.d0    Mg(OH)2                     Brucite    CRC p.B-181:185
18      2.d3    Na6CO3(SO4)2                Burkeite
19   2828.d0    CaCO3                       Calcite    CRC p.B-181:185
20      2.d3    CaCl2.4H2O       CaCl2 Tetrahydrite
21      2.d3    Ca4Cl2(OH)6.13H2O  CaOxychloride A
22      2.d3    Ca2Cl2(OH)2.H2O    CaOxychloride B
23   1602.d0    KMgCl3.6H2O                 Carnallite CRC p.B-181:185
24   1677.d0    MgSO4.7H2O                  Epsomite   CRC p.B-181:185
25   1991.d0    CaNa2(CO3)2.5H2O            Gaylussite CRC p.B-181:185
26   2800.d0    Na2Ca(SO4)2                 Glauberite CRC p.B-181:185
27   2335.d0    CaSO4.2H2O                  Gypsum     CRC p.B-181:185
28   2165.d0    NaCl                        Halite     CRC p.B-181:185
29      2.d3    MgSO4.6H2O                Hexahydrite
30   2150.d0    KMgClSO4.3H2O               Kainite    CRC p.B-181:185
31      2.d3    KHCO3                     Kalicinite
32   2571.d0    MgSO4.H2O                   Kieserite  CRC p.B-181:185
33      2.d3    K2Mg(SO4)2.4H2O             Leonite
34      2.d3    Na4Ca(SO4)3.2H2O         Labile Salt
35   3210.d0    MgCO3                       Magnesite  CRC p.B-181:185
36      2.d3    Mg2Cl(OH)3.4H2O         MgOxychloride
37      2.d3    KHSO4                     Mercallite
38   1490.d0    Na2SO4.10H2O                Mirabilite CRC p.B-181:185
39      2.d3    K8H6(SO4)7                  Misenite
40      2.d3    NaHCO3                    Nahcolite
41      2.d3    Na2CO3.10H2O                Natron
42      2.d3    MgCO3.3H2O              Nesquehonite
43      2.d3    K2Mg(SO4)2.6H2O  Picromerite/Schoen
44      2.d3    Na2Ca(CO3)2.2H2O            Pirssonite
45      2.d3    K2MgCa2(SO4)4.2H2O          Polyhalite
46      2.d3    Ca(OH)2                   Portlandite
47      2.d3    K2CO3.3/2H2O    Potassium Carbonate
48      2.d3    K8H4(CO3)6.3H2O   K-Sequicarbonate
49      2.d3    KNaCO3.6H2O         K-Na-Carbonate
50      2.d3    K2NaH(CO3)2.2H2O   Potassium Trona
51      2.d3    K3H(SO4)2  Sesquipotassium Sulfate
52      2.d3    Na3H(SO4)2     Sesquisodium Sulfate
53      2.d3    Na2CO3.7H2O    Na2CO3-Heptahydrate
54   1990.d0    KCl                         Sylvite    CRC p.B-181:185
55      2.d3    K2Ca(SO4)2.H2O              Syngenite
56      2.d3    Mg2CaCl6.12H2O           Tachyhydrite
57      2.d3    Na2SO4                     Thenardite
58   2255.d0    Na2CO3.H2O                Thermonatrite CRC p.B-181:185
59   2140.d0    Na3H(CO3)2.2H2O                Trona     CRC p.B-181:185
60   1715.d0    Na2B4O7.10H2O                  Borax     CRC p.B-181:185
61      2.d3    B(OH)3                Borix Acid Solid
62      2.d3    KB5O8.4H2O     K-Pentaborate (30 C)
63      2.d3    K2B4O7.4H2O    K-Tetraborate (30 C)
64      2.d3    NaBO2.4H2O       Sodium Metaborate
65      2.d3    NaB5O8.5H2O      Sodium Pentaborate
66      2.d3    NaBO2.NaCl.2H2O   Teepleite (20 C)
```

K.2 References Cited in Listing

Novak, C.F. 1994. "Development of the FMT Chemical Transport Simulator: Coupling Aqueous Density and Mineral Volume Fraction to Phase Composition." *Proceedings of the Fourth International Conference on the Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere* . Special Issue of Radiochimica Acta. R. Oldenbourg Verlag: München, Germany.

Weast, R.C. 1980. *CRC Handbook of Chemistry and Physics* 60th ed. Chemical Rubber Publishing Company, Boca Raton, Florida.

Appendix L: Sample Output File "BATCH_DOC.OUT"

See Table 14 for explanation of this listing.

```
INPUT    file name is:U1:[SCBARB.FMT.UM]BATCH_DOC.IN;1
INGUESS  file name is:U1:[SCBARB.FMT.UM]BATCH_DOC.INGUESS;1
OUTPUT   file name is:U1:[SCBARB.FMT.UM]BATCH_DOC.OUT;1
CHEMDAT  file name is U1:[SCBARB.FMT.UM]FMT_HNW_NP_AM_RTEST.CHEMDAT;1
Temperature is Hard Coded as 298.15K
(.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs                FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

*******************************************************************************
*** ECHO PRINT OF 'CHEMDAT' FILE WOULD BE HERE ***
***            SEE APPENDIX J                   ***
*******************************************************************************

Will calculate gamma for BJO3(OH)4-              BJO3(OH)4-
Will calculate gamma for B4O5(OH)4=              B4O5(OH)4=
Will calculate gamma for HCl(aq).....to.titrate.acid.only
Will calculate gamma for NaOH(aq)......to.titrate.base.only

************SOLUBILITY PRODUCT VIOLATION*************
** Mg(OH)2_____________________Brucite **  1.00E+01 **

************SOLUBILITY PRODUCT VIOLATION*************
** Mg2Cl(OH)3.4H2O_____MgOxychloride **  6.69E+00 **

          2 Solubility Product Violations
Adding solid Mg(OH)2_____________________Brucite
# inversions for batch pblm          84
1(.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs              FMT V2.3
 DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality     Aq. Molarity     Aq. mg/liter

Using NaCl Density Correlation
  1.10222364E+02   1.11116160E+02   1.10794086E+02   1.11669359E+05  Hydrogen
  5.51654821E+01   5.56118135E+01   5.54506206E+01   8.87176659E+05  Oxygen
  2.00000000E-01   2.01625464E-01   2.01041045E-01   4.62188739E+03  Sodium
  1.00000000E-02   1.00812732E-02   1.00520523E-02   3.93018155E+02  Potassium
  1.00000000E-03   4.66737768E-08   4.63326894E-08   1.12611601E-03  Magnesium
  1.00000000E-04   1.00812732E-04   1.00520523E-04   4.02886254E+00  Calcium
  1.10000000E-01   1.10894005E-01   1.10572575E-01   3.92012950E+03  Chlorine
  1.00000000E-03   1.00812732E-03   1.00520523E-03   3.22268795E+01  Sulfur
  1.00000000E-04   1.00812732E-04   1.00520523E-04   1.20735200E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  1.00000000E-07   1.00812732E-07   1.00520523E-07   1.08662685E-03  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
  1.11805846E-16   1.12714528E-16   1.12387821E-16   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     1002.59976105542      grams
    H2O MASS          991.938201296740      grams
    TDS(g/kg)         10.7482096613920      g/kgH2O

  Specified Solution Density
    DENSITY           1007.81851904202      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL   0.9946217284282B5        liters
    TDS               10.7170555829390      g/l

  Density based on TDS and NaCl solutions     1007.81851904202      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                          Molality     Activity     Act Coef     Total Moles   Molarity     mg/liter     Descriptor
H2O                        WATER      9.92444E-01  9.93023E-01   1.001       5.50612E+01  5.53478E+01  9.97101E+05
Na+                          Na+      2.01625E-01  1.47085E-01   0.7295      2.00000E-01  2.01041E-01  4.62189E+03
Cl-                          Cl-      1.10894E-01  7.98916E-02   0.7204      1.10000E-01  1.10573E-01  3.92013E+03
OH-                          OH-      9.87965E-02  7.13751E-02   0.7224      9.80001E-02  9.85102E-02  1.67539E+03
K+                           K+       1.00813E-02  7.34149E-03   0.7282      1.00000E-02  1.00521E-02  3.93018E+02
SO4=                         SO4=     1.00813E-03  2.24998E-04   0.2232      1.00000E-03  1.00521E-03  9.65576E+01
Mg(OH)2_____________Brucite  Brucite  1.00808E-03  1.00000E+00   1.000       9.99954E-04  1.00516E-03  5.86205E+01
Ca++                         Ca++     1.00115E-04  2.00966E-05   0.2007      9.93083E-05  9.98252E-05  4.00099E+00
CO3=                         CO3=     1.00005E-04  2.44915E-05   0.2449      9.91991E-05  9.97155E-05  5.98385E+00
B(OH)4-                      B(OH)4-  1.00709E-07  6.61270E-08   0.6566      9.98971E-08  1.00417E-07  7.91680E-03
Mg++                         Mg++     1.09873E-08  2.56221E-09   0.2332      1.08986E-08  1.09555E-08  2.66273E-04   2.12E-10
MgOH+                        MgOH+    3.54268E-08  2.81647E-08   0.7950      3.51412E-08  3.53241E-08  1.45932E-03  -2.00E-07
MgCO3(aq)                    MgCO3(aq)  5.32206E-11  5.32206E-11   1.000     5.27915E-11  5.30663E-11  4.47424E-06   2.82E-10
CaCO3(aq)                    CaCO3(aq)  6.97236E-07  6.97236E-07   1.000     6.91615E-07  6.95215E-07  6.95835E-02   1.24E-10
HCO3-                        HCO3-    1.10094E-07  7.49923E-08   0.6812      1.09206E-07  1.09775E-07  6.69815E-03   1.42E-10
MgB(OH)4+                    MgB(OH)4+  6.18470E-15  4.24905E-15  0.6870     6.13484E-15  6.16677E-15  6.36066E-10   2.66E-10
CaB(OH)4+                    CaB(OH)4+  8.72370E-11  5.94047E-11  0.6810     8.65337E-11  8.69841E-11  1.03441E-05   3.28E-11
B(OH)3(aq)                   B(OH)3(aq)  1.65411E-11  1.61858E-11  0.9785     1.64077E-11  1.64931E-11  1.01980E-06   1.46E-10
H+                           H+       1.93212E-13  1.40201E-13   0.7256      1.91654E-13  1.92652E-13  1.94173E-10   1.23E-10
CO2(aq)                      CO2(aq)  2.21142E-14  2.30277E-14   1.041       2.19360E-14  2.20501E-14  9.70422E-10   2.82E-10
HSO4-                        HSO4-    4.06799E-15  3.00314E-15   0.7382      4.03519E-15  4.05620E-15  3.93717E-10   1.83E-10
K6H4(CO3)6.3H2O___K-Sequicarbonate  0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -6.18E+01
NaB5O8.5H2O_____Sodium_Pentaborate  0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -4.78E+01
NaBO2.NaCl.2H2O___Teepleite_(20_C)  0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.15E+01
CaSO4_____________Anhydrite         0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.98E+00
NaK3(SO4)2___Aphthitalite/Glaserite  0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.07E+01
CaCl2.6H2O_____________Antarcticite  0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.11E+01
CaCO3_____________Aragonite         0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.09E+00
KJSO4_____________Arcanite          0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -6.14E+00
MgCl2.6H2O_____________Bischofite   0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.53E+01
Na2Mg(SO4)2.4H2O_____Bloedite       0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.52E+01
```

Appendix L: Sample Output File "BATCH_DOC.OUT"

Na6CO3(SO4)2	Burkeite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.61E+01
CaCO3	Calcite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.02E-01
CaCl2.4H2O	CaCl2_Tetrahydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.26E+01
Ca2Cl2(OH)2.H2O	CaOxychloride B	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E+01
KMgCl3.6H2O	Carnallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.84E+01
MgSO4.7H2O	Epsomite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.04E+01
CaNa2(CO3)2.5H2O	Gaylussite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.16E+00
Na2Ca(SO4)2	Glauberite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.41E+00
CaSO4.2H2O	Gypsum	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.77E+00
NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.50E+00
MgSO4.6H2O	Hexahydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.06E+01
KMgClSO4.3H2O	Kainite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.53E+01
KHCO3	Kalicinite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.54E+00
MgSO4.H2O	Kieserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.21E+01
K2Mg(SO4)2.4H2O	Leonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+01
Na4Ca(SO4)3.2H2O	Labile_Salt	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.33E+01
MgCO3	Magnesite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.37E+00
Mg2Cl(OH)3.4H2O	MgOxychloride	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.77E+00
KHSO4	Mercallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.58E+01
Na2SO4.10H2O	Mirabilite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.72E+01
NaBO2.4H2O	Sodium_Metaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.12E+00
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.35E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.48E+00
MgCO3.3H2O	Nesquahonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.04E+00
K2Mg(SO4)2.6H2O	Picromerite/Schoen	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.58E+01
Na2Ca(CO3)2.2H2O	Pirssonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.35E+00
K2MgCa2(SO4)4.2H2O	Polyhalite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.31E+01
Ca(OH)2	Portlandite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.80E+00
K2CO3.3/2H2O	Potassium_Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.19E+01
KNaCO3.6H2O	K-Na-Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.46E+00
K2NaH(CO3)2.2H2O	Potassium_Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.81E+01
K3H(SO4)2	Sesquipotassium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+01
Na3H(SO4)2	Sesquisodium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.16E+01
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.64E+00
KCl	Sylvite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.13E+00
K2Ca(SO4)2.H2O	Syngenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.82E+00
Mg2CaCl6.12H2O	Tschyhydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.59E+01
Na2SO4	Thenardite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.03E+00
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.76E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.32E+01
Na2B4O7.10H2O	Borax	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.16E+01
B(OH)3	Borix_Acid_Solid	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.08E+01
KB5O8.4H2O	K-Pentaborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.79E+01
K2B4O7.4H2O	K-Tetraborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.56E+01
KBH6(SO4)7	Misenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+02
Ca4Cl2(OH)6.13H2O	CaOxychloride A	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.27E+01
NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.93E+02
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.54E+02
B4O5(OH)4-	B4O5(OH)4-	0.00000E+00	0.00000E+00	2.8441E-02	0.00000E+00	0.00000E+00	0.00000E+00	-3.36E+01
B3O3(OH)4-	B3O3(OH)4-	0.00000E+00	0.00000E+00	0.3248	0.00000E+00	0.00000E+00	0.00000E+00	-2.70E+01

pH (-log[aH+]); pmH(-log[mH+]) 12.8532 12.7140
Osmotic Coefficient= 0.919612
Equilibrium RH (%) = 99.302313
Ionic Strength (m) = 0.213115
Density, kg/m3 = 1007.82
fCO2(g); log(fCO2(g))= 6.983E-13 -12.2

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
"dG/RT/ln10 for species with nonzero concs. (convergence criterion)
"Saturation Index for minerals, SI=log10(IAP/Ksp)
"log10(activity) for aqueous species with very small concentrations
"log10(partial pressure) for gases

Total G/RT= -5.30370149E+03

Total Diagonal Inversions 84
Total Stoichiometric Reoptimizations 9

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

See Table 15 for explanation of this listing.

```
INPUT    file name is:U1:[SCRABB.FMT.UM]NP_NACL_BM_LOG.IN;1
INGUESS  file name is:U1:[SCRABB.FMT.UM]NP_NACL_BM_LOG.INGUESS;1
OUTPUT   file name is:U1:[SCRABB.FMT.UM]NP_NACL_BM_LOG.OUT;1
CHEMDAT  file name is U1:[SCRABB.FMT.UM]FMT_MRM_NP_AM_RTEST.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)

Accuracy of reactions is            1.0000E-06
Minimum elemental abundance is      1.0000E-18
Number of Aqueous Species is        50

PITZER Data Base NOT Echoed in this Run

Species Order for Pitzer Parameters

Cations    13

Na+              K+               Ca++             Mg++             MgOH+            H+
MgB(OH)4+        CaB(OH)4+        Am+++            AmCO3+           Th++++           UO2++
NpO2+

Anions     20

Cl-              SO4=             HSO4-            OH-              HCO3-            CO3=
B(OH)4-          B3O3(OH)4-       B4O5(OH)4=       Br-              Am(CO3)2-        Am(CO3)3=-
ClO4-            pe NpO2(OH)2-    NpO2CO3-         NpO2(CO3)2=-     NpO2(CO3)3=-=-   H2PO4-
HPO4=            PO4=-

Neutral    6

CO2(aq)          CaCO3(aq)        MgCO3(aq)        B(OH)3(aq)       NpO2OH(aq)       H3PO4(aq)

using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

this is a TITRATION problem

Ideal Gas Constant is Unity (Dimensionless)
Temperature =       298.15 [=] degree Kelvin

  115 Species                    23 Elements

        Element Name        Molecular Weight
        Hydrogen                   1.00790
        Oxygen                    15.99940
        Sodium                    22.98977
        Potassium                 39.09830
        Magnesium                 24.30500
        Calcium                   40.08000
        Chlorine                  35.45300
        Sulfur                    32.06000
        Carbon                    12.01100
        PosIon                     0.00000
        NegIon                     0.00000
        Air                       28.84000
        Boron                     10.81000
        Bromine                   79.90400
        TracerEl                   0.00000
        Th(IV)                   232.03810
        Am(III)                  243.00000
        U(VI)                    238.02900
        Np(V)                    237.04820
        ClO4-(EL)                 99.45060
        Phosphorus                30.97400
        Electron                   0.00000
        Charge                     0.00000

   Species Name                              Phase      Mol.Wt.    Std Chemical Potential, u/RT
 1 H2O                                 WATER  aqueous    18.015      -95.6635
 2 Na+                                   Na+  aqueous    22.990     -105.6510
 3 K+                                     K+  aqueous    39.098     -113.9570
 4 Ca++                                 Ca++  aqueous    40.080     -223.3000
 5 Mg++                                 Mg++  aqueous    24.305     -183.4680
 6 MgOH+                               MgOH+  aqueous    41.312     -251.9400
 7 H+                                     H+  aqueous     1.008        0.0000
 8 Cl-                                   Cl-  aqueous    35.453      -52.9550
 9 SO4=                                 SO4=  aqueous    96.058     -300.3860
10 HSO4-                               HSO4-  aqueous    97.066     -304.9420
11 OH-                                   OH-  aqueous    17.007      -63.4350
12 HCO3-                               HCO3-  aqueous    61.017     -236.7510
13 CO3=                                 CO3=  aqueous    60.009     -212.9440
14 CO2(aq)                           CO2(aq)  aqueous    44.010     -155.6800
15 CaCO3(aq)                       CaCO3(aq)  aqueous   100.089     -443.5000
16 MgCO3(aq)                       MgCO3(aq)  aqueous    84.314     -403.1550
17 B(OH)3(aq)                      B(OH)3(aq)  aqueous    61.832     -390.8100
18 B(OH)4-                           B(OH)4-  aqueous    78.839     -465.2000
19 B3O3(OH)4-                      B3O3(OH)4-  aqueous   148.457     -963.7700
20 B4O5(OH)4=                      B4O5(OH)4=  aqueous   191.266    -1239.1000
21 CaB(OH)4+                       CaB(OH)4+  aqueous   118.919     -692.3000
22 MgB(OH)4+                       MgB(OH)4+  aqueous   103.144     -651.8900
23 Br-                                   Br-  aqueous    79.904     -999.9900
24 ClO4-                 perchlorate ClO4-  aqueous    99.451     -999.9900
25 NaOH(aq).....to.titrate.base.only       aqueous    39.997      500.0000
26 HCl(aq).....to.titrate.acid.only        aqueous    36.461      500.0000
27 HClO4(aq).....to.titrate.acid.only      aqueous   100.459      500.0000
28 PosIon.................POSITIVE.ION     aqueous     0.000        0.0000
29 NegIon.................NEGATIVE.ION     aqueous     0.000        0.0000
30 PosIon(OH)(aq).....to.titrate.base      aqueous    17.007      500.0000
31 HNegIon(aq).....to.titrate.acid         aqueous     1.008      500.0000
32 Tracer(aq).....conservative.tracer      aqueous     0.000        0.0000
33 H3PO4(aq)                       H3PO4(aq)  aqueous    97.995     -460.9000
34 H2PO4-                           H2PO4-  aqueous    96.987     -455.9600
35 HPO4=                             HPO4=  aqueous    95.980     -439.3670
36 PO4=-                             PO4=-  aqueous    94.972     -410.9470
37 NpO2+                             NpO2+  aqueous   269.047     -369.1270
38 NpO2OH(aq)                   NpO2OH(aq)  aqueous   286.054     -438.5180
39 NpO2(OH)2-                   NpO2(OH)2-  aqueous   303.062     -505.8290
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

115	40	NpO2CO3-	NpO2CO3-	aqueous	329.056	-594.4920	
116	41	NpO2(CO3)2=-	NpO2(CO3)2=-	aqueous	389.065	-808.4010	
117	42	NpO2(CO3)3=5-	NpO2(CO3)3=5-	aqueous	449.075	-1019.9180	
118	43	Am+++	Am+++	aqueous	243.000	-241.6940	
119	44	AmCO3+	AmCO3+	aqueous	303.009	-472.0600	
120	45	Am(CO3)2-	Am(CO3)2-	aqueous	363.018	-695.8800	
121	46	Am(CO3)3=-	Am(CO3)3=-	aqueous	423.028	-915.4600	
122	47	Am(OH)2+	Am(OH)2+	aqueous	277.015	-393.6470	
123	48	Am(OH)3(aq)	Am(OH)3(aq)	aqueous	294.022	-462.9500	
124	49	Th++++	Th++++	aqueous	232.038	-999.9900	
125	50	UO2++	U(VI)O2++	aqueous	270.028	-999.9900	
126	51	NpO2OH(aged)	NpO2OH(aged)	solid	286.054	-454.0100	
127	52	NpO2OH(amor)	NpO2OH(amor)	solid	286.054	-452.6420	
128	53	NaNpO2CO3(s)	NaNpO2CO3(s)	solid	352.046	-711.7070	
129	54	NaJNpO2(CO3)2(s)	DISABLED_DISABLED	solid	458.035	999.9900	
130	55	AmOHCO3(c)	AmOHCO3(c)	solid	320.017	-569.9800	
131	56	Am(OH)3(s)	Am(OH)3(s)	solid	294.022	-492.2940	
132	57	NaAm(CO3)2.6H2O(c)		solid	494.099	-1396.4940	
133	58	AmPO4(c)	AmPO4(c)	solid	337.972	-709.7500	
134	59	CaSO4	Anhydrite	solid	136.138	-533.7300	
135	60	NaK3(SO4)2	Aphthitalite/Glaserite	solid	332.400	-1057.0500	
136	61	CaCl2.6H2O	Antarcticite	solid	219.077	-893.6500	
137	62	CaCO3	Aragonite	solid	100.089	-455.1700	
138	63	K2SO4	Arcanite	solid	174.254	-532.3900	
139	64	MgCl2.6H2O	Bischofite	solid	203.302	-853.1000	
140	65	Na2Mg(SO4)2.4H2O	Bloedite	solid	334.461	-1383.6000	
141	66	Mg(OH)2	Brucite	solid	58.320	-335.4000	
142	67	Na6CO3(SO4)2	Burkeite	solid	390.063	-1449.4000	
143	68	CaCO3	Calcite	solid	100.089	-455.6000	
144	69	CaCl2.4H2O	CaCl2_Tetrahydrite	solid	183.047	-698.7000	
145	70	Ca4Cl2(OH)6.13H2O	CaOxychloride A	solid	567.467	-2658.4500	
146	71	Ca2Cl2(OH)2.H2O	CaOxychloride B	solid	203.096	-778.4100	
147	72	KMgCl3.6H2O	Carnallite	solid	277.854	-1020.3000	
148	73	MgSO4.7H2O	Epsomite	solid	246.469	-1157.8300	
149	74	CaNa2(CO3)2.5H2O	Gaylussite	solid	296.154	-1360.5000	
150	75	Na2Ca(SO4)2	Glauberite	solid	278.175	-1047.4500	
151	76	CaSO4.2H2O	Gypsum	solid	172.168	-725.5600	
152	77	NaCl	Halite	solid	58.443	-154.9900	
153	78	MgSO4.6H2O	Hexahydrite	solid	228.454	-1061.6000	
154	79	KMgClSO4.3H2O	Kainite	solid	248.960	-938.2000	
155	80	KHCO3	Kalicinite	solid	100.115	-350.0600	
156	81	MgSO4.H2O	Kieserite	solid	138.378	-579.8000	
157	82	K2Mg(SO4)2.4H2O	Leonite	solid	366.678	-1403.9700	
158	83	Na4Ca(SO4)3.2H2O	Labile_Salt	solid	456.242	-1751.4500	
159	84	MgCO3	Magnesite	solid	84.314	-414.4500	
160	85	Mg2Cl(OH)3.4H2O	MgOxychloride	solid	207.146	-1029.6000	
161	86	KHSO4	Mercallite	solid	136.164	-417.5700	
162	87	Na2SO4.10H2O	Mirabilite	solid	322.189	-1471.1500	
163	88	K8H6(SO4)7	Misenite	solid	991.237	-3039.2400	
164	89	NaHCO3	Nahcolite	solid	84.007	-343.3300	
165	90	Na2CO3.10H2O	Natron	solid	286.141	-1382.7800	
166	91	MgCO3.3H2O	Nesquehonite	solid	138.360	-695.3000	
167	92	K2Mg(SO4)2.6H2O	Picromerite/Schoen	solid	402.708	-1596.1000	
168	93	Na2Ca(CO3)2.2H2O	Pirssonite	solid	242.108	-1073.1000	
169	94	K2MgCa2(SO4)4.2H2O	Polyhalite	solid	602.922	-2282.5000	
170	95	Ca(OH)2	Portlandite	solid	74.095	-362.1200	
171	96	K2CO3.3/2H2O	Potassium_Carbonate	solid	165.229	-577.3700	
172	97	K8H6(CO3)6.3H2O	K-Sequicarbonate	solid	730.919	-2555.4000	
173	98	KNaCO3.6H2O	K-Na-Carbonate	solid	230.188	-1006.8000	
174	99	K2NaH(CO3)2.2H2O	Potassium_Trona	solid	258.243	-971.7400	
175	100	K3H(SO4)2	Sesquipotassium_Sulfate	solid	310.418	-950.8000	
176	101	Na3H(SO4)2	Sesquisodium_Sulfate	solid	262.092	-919.6000	
177	102	Na2CO3.7H2O	Na2CO3-Heptahydrate	solid	232.095	-1094.9500	
178	103	KCl	Sylvite	solid	74.551	-164.8400	
179	104	K2Ca(SO4)2.H2O	Syngenite	solid	328.407	-1164.8000	
180	105	Mg2CaCl6.12H2O	Tachyhydrite	solid	517.590	-2015.9000	
181	106	Na2SO4	Thenardite	solid	142.037	-512.3500	
182	107	Na2CO3.H2O	Thermonatrite	solid	124.004	-518.8000	
183	108	Na3H(CO3)2.2H2O	Trona	solid	226.026	-960.3800	
184	109	Na2B4O7.10H2O	Borax	solid	381.367	-2224.1600	
185	110	B(OH)3	Borix_Acid_Solid	solid	61.832	-390.8800	
186	111	KB5O8.4H2O	K-Pentaborate_(30_C)	solid	293.204	-1770.2600	
187	112	K2B4O7.4H2O	K-Tetraborate_(30_C)	solid	305.493	-1663.4700	
188	113	NaBO2.4H2O	Sodium_Metaborate	solid	137.859	-761.4200	
189	114	NaB5O8.5H2O	Sodium_Pentaborate	solid	295.111	-1854.8000	
190	115	NaBO2.NaCl.2H2O	Teepleite_(20_C)	solid	160.272	-725.7700	
191							
192							

		Truncated Name	Formula Matrix																							
193																										
194	1	H2O	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
195	2	Na+	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
196	3	K+	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
197	4	Ca++	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
198	5	Mg++	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
199	6	MgOH+	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
200	7	H+	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
201	8	Cl-	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
202	9	SO4=	0	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2
203	10	HSO4-	1	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
204	11	OH-	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
205	12	HCO3-	1	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
206	13	CO3=	0	3	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	-2
207	14	CO2(aq)	0	2	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
208	15	CaCO3(aq)	0	3	0	0	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
209	16	MgCO3(aq)	0	3	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
210	17	B(OH)3(aq)	3	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
211	18	B(OH)4-	4	4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
212	19	B3O3(OH)4-	4	7	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	-1
213	20	B4O5(OH)4=	4	9	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	-2
214	21	CaB(OH)4+	4	4	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
215	22	MgB(OH)4+	4	4	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
216	23	Br-	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-1
217	24	ClO4- pe	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1
218	25	NaOH(aq).....to,ti	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
219	26	HCl(aq).....to,ti	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
220	27	HClO4(aq).....to,ti	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
221	28	PosIon.....	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1
222	29	NegIon.....	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	-1
223	30	PosIon(OH)(aq).....	1	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
224	31	NNegIon(aq).....	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
225	32	Tracer(aq).....cons	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
226	33	H3PO4(aq)	3	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
227	34	H2PO4-	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1
228	35	HPO4=	1	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-2
229	36	PO4=-	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-3
230	37	NpO2+	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
231	38	NpO2OH(aq)	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
232	39	NpO2(OH)2-	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-1
233	40	NpO2CO3-	0	5	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-1
234	41	NpO2(CO3)2=-	0	8	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-3
235	42	NpO2(CO3)3=5-	0	11	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-5
236	43	Am+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	3
237	44	AmCO3+	0	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1
238	45	Am(CO3)2-	0	6	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	-1

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  46 Am(CO3)3---          0  9  0  0  0  0  0  0  3  0  0  0  0  0  0  0  1  0  0  0  0  0 -3
  47 Am(OH)2+             2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  1
  48 Am(OH)3(aq)          3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0
  49 Th++++               0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  4
  50 UO2++                0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  2
  51 NpO2OH(aged)_______  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0
  52 NpO2OH(amor)_______  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0
  53 NaNpO2CO3(s)_______  0  5  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  1  0  0  0  0
  54 Na3NpO2(CO3)2(s)_DI  0  8  3  0  0  0  0  0  2  0  0  0  0  0  0  0  0  1  0  0  0  0
  55 AmOHCO3(c)_________  1  4  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  1  0  0  0  0
  56 Am(OH)3(s)_________  3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
  57 NaAm(CO3)2.6H2O(c)_ 12 12  1  0  0  0  0  0  2  0  0  0  0  0  0  0  0  1  0  0  0  0
  58 AmPO4(c)___________  0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0
  59 CaSO4______________  0  4  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  1  0  0  0  0
  60 NaK3(SO4)2__Aphthit  0  8  1  3  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  61 CaCl2.6H2O_________ 12  6  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  62 CaCO3______________  0  3  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  63 K2SO4______________  0  4  0  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  64 MgCl2.6H2O_________ 12  6  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  65 Na2Mg(SO4)2.4H2O___  8 12  2  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  66 Mg(OH)2____________  2  2  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  67 Na6CO3(SO4)2_______  0 11  6  0  0  0  0  2  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  68 CaCO3______________  0  3  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  69 CaCl2.4H2O_____CaC  8  4  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  70 Ca4Cl2(OH)6.13H2O__ 32 19  0  0  0  4  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  71 Ca2Cl2(OH)2.H2O____  4  3  0  0  0  2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  72 KMgCl3.6H2O________ 12  6  0  1  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  73 MgSO4.7H2O_________ 14 11  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  74 CaNa2(CO3)2.5H2O___ 10 11  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0
  75 Na2Ca(SO4)2________  0  8  2  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  76 CaSO4.2H2O_________  4  6  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  77 NaCl_______________  0  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  78 MgSO4.6H2O_________ 12 10  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  79 KMgClSO4.3H2O______  6  7  0  1  1  0  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  80 KHCO3______________  1  3  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  81 MgSO4.H2O__________  2  5  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  82 K2Mg(SO4)2.4H2O____  8 12  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  83 Na4Ca(SO4)3.2H2O___  4 14  4  0  0  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  84 MgCO3______________  0  3  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  85 Mg2Cl(OH)3.4H2O____ 11  7  0  0  2  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  86 KHSO4______________  1  4  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  87 Na2SO4.10H2O_______ 20 14  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  88 K8H6(SO4)7_________  6 28  0  8  0  0  0  7  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  89 NaHCO3_____________  1  3  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  90 Na2CO3.10H2O_______ 20 13  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  91 MgCO3.3H2O_________  6  6  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  92 K2Mg(SO4)2.6H2O Pic 12 14  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  93 Na2Ca(CO3)2.2H2O___  4  8  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0
  94 K2MgCa2(SO4)4.2H2O_  4 18  0  2  1  2  0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  95 Ca(OH)2____________  2  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  96 K2CO3.3/2H2O___Pota  3  4  0  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  97 K8H4(CO3)6.3H2O___K 10 21  0  8  0  0  0  0  6  0  0  0  0  0  0  0  0  0  0  0  0  0
  98 KNaCO3.6H2O________ 12  9  1  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
  99 K2NaH(CO3)2.2H2O___  5  8  1  2  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0
 100 K3H(SO4)2__Sesquipo  1  8  0  3  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 101 Na3H(SO4)2____Sesqu  1  8  3  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 102 Na2CO3.7H2O____Na2C 14 10  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
 103 KCl_______________  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 104 K2Ca(SO4)2.H2O_____  2  9  0  2  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 105 MgCaCl6.12H2O______ 24 12  0  0  2  1  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 106 Na2SO4____________  0  4  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 107 Na2CO3.H2O________  2  4  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
 108 Na3H(CO3)2.2H2O____  5  8  3  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0
 109 Na2B4O7.10H2O______ 20 17  2  0  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0
 110 B(OH)3_____________B  3  3  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0
 111 KB5O8.4H2O____K-Pen  8 12  0  1  0  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0
 112 K2B4O7.4H2O___K-Tet  8 11  0  2  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0
 113 NaBO2.4H2O_________So  8  6  1  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0
 114 NaB5O8.5H2O_____Sod 10 13  1  0  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0
 115 NaBO2.NaCl.2H2O___T  4  4  2  0  0  0  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0
 ************************************************************************************************************************

RHOMIN    file name is U1:[SCBARB.FMT.UM]FMT_HMM_NP_AM_RTEST.RHOMIN;1
 # inversions for batch pblm          56
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl    FMT V2.3
DATABASE:  NEMB4/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

   Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

   1.11017363E+02    1.11029658E+02    1.00100314E+02    1.00891107E+05  Hydrogen
   6.15086815E+01    6.15154934E+01    5.54601388E+01    8.87328944E+05  Oxygen
   5.61000000E+00    5.61062139E+00    5.05833276E+00    1.16289907E+05  Sodium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
   1.61000000E+00    1.61017838E+00    1.45167838E+00    5.14663538E+04  Chlorine
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
   2.00000001E+00    2.00022150E+00    1.80332719E+00    2.16597629E+04  Carbon
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  PosIon
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  NegIon
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Th(IV)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Np(V)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
  -1.77635684E-15   -1.77655356E-15   -1.60167629E-15    0.00000000E+00  Charge

   Solution Parameters, Calculated
     SOLUTION MASS      1306.07033909890       grams
     H2O MASS           999.889265717486       grams
     TDS(g/kg)          306.214981677726       g/kgH2O

   Specified Solution Density
     DENSITY            1177.63607439302       kg/m^3 = g/l

   Solution Parameters Based on Specified Density
     SOLUTION VOL       1.10906108219560       liters
     TDS                276.072326670473       g/l

   Density based on TDS and NaCl solutions     1177.63607439302      g/l
   Percent relative error vs NaCl density    0.000000000000000E+000 %
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                  WATER    8.57464E-01   8.59843E-01    1.003        5.55025E+01   5.00446E+01   9.01564E+05
Na+                                    Na+    5.61062E+00   3.69881E+00   0.6593        5.61000E+00   5.05833E+00   1.16290E+05
CO3=                                   CO3=   1.99407E+00   4.09214E-02   2.0522E-02    1.99385E+00   1.79778E+00   1.07884E+05
Cl-                                    Cl-    1.61018E+00   1.06477E+00   0.6613        1.61000E+00   1.45168E+00   5.14664E+04
HCO3-                                  HCO3-  6.14734E-03   1.59044E-03   0.2587        6.14666E-03   5.54222E-03   3.38170E+02
OH-                                    OH-    6.14733E-03   6.86901E-03   0.7921        6.14665E-03   5.54221E-03   9.42580E+01    2.07E-11
CO2(aq)                             CO2(aq)   2.36876E-09   7.15913E-09   3.022         2.36850E-09   2.13559E-09   9.39866E-05   -2.10E-07
H+                                     H+     2.39954E-12   1.77959E-12   0.7416        2.39927E-12   2.16344E-12   2.18043E-09   -8.49E-08
HCl(aq).....to.titrate.acid.only               0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+02
NaOH(aq).....to.titrate.base.only              0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.92E+02
Na2CO3.10H2O_____________Natron                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.30E-02
Na2CO3.H2O_____Thermonatrite                   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.99E-01
Na2CO3.7H2O____Na2CO3-Heptahydrate             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.51E-01
NaHCO3_____________Nahcolite                   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.83E+00
NaCl_____________Halite                        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.75E-01
Na3H(CO3)2.2H2O_____________Trona              0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.57E+00

pH (-log[aH+]); pmH(-log[mH+])      11.7497      11.6199
Osmotic Coefficient=     0.908418
Equilibrium RH (%) =    85.984284
Ionic Strength (m) =     7.606695
Density, kg/m3     =     1177.64
fCO2(g); log[fCO2(g)]=                                    2.171E-07    -6.66

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *d2/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -6.42133776E+03

Reaction #            1 aldaum     2.00000000000000
This is a solid-only reaction

shifting left by     4.64434654478256
calling makenuv for allomorphic reactions
# inversions for batch pblm          99
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.6imolal NaCl   FMT V2.3
 DATABASE:  NMM96/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFRR92,RFP94,RRFP94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

  1.11018163E+02    1.11017591E+02    9.91838868E+01    1.00169020E+05   Hydrogen
  1.05508682E+02    5.55113597E+01    4.96942389E+01    7.95078006E+05   Oxygen
  1.56100000E+01    5.61057382E+00    5.02263116E+00    1.15469161E+05   Sodium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Potassium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Magnesium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Calcium
  5.61100000E+00    5.61096098E+00    5.02297975E+00    1.78079701E+05   Chlorine
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Sulfur
  1.00000000E+01    6.12839260E-04    5.48618892E-04    6.58946151E+00   Carbon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   PosIon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   NegIon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Air
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Boron
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Bromine
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   TracerEl
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Th(IV)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   As(III)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   U(VI)
  1.00000000E+01    6.12839260E-04    5.48618892E-04    1.30049121E+02   Np(V)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   ClO4-(EL)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Phosphorus
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Electron
 -4.28740972E-15   -4.28737990E-15   -3.83809877E-15    0.00000000E+00   Charge

  Solution Parameters, Calculated
    SOLUTION MASS      1328.11614865108      grams
    H2O MASS           1000.00695466820      grams
    TDS(g/kg)          328.106912108174      g/kgH2O

  Specified Solution Density
    DENSITY            1188.93254605458      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL       1.11706602116190      liters
    TDS                293.724084133903      g/l

  Density based on TDS and NaCl solutions     1188.93254605458      g/l
  Percent relative error vs NaCl density      0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                  WATER    8.31822E-01   7.77959E-01   0.9352        5.55091E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)         9.99332E+00   1.00000E+00    1.000        9.99939E+00   8.95147E+00   3.15133E+06
Cl-                                    Cl-    5.61096E+00   5.29329E+00   0.9434        5.61100E+00   5.02298E+00   1.78080E+05
Na+                                    Na+    5.61057E+00   5.29268E+00   0.9433        5.61061E+00   5.02263E+00   1.15469E+05
NpO2+                                  NpO2+  6.12705E-04   1.31978E-03   1.991         6.12709E-04   5.48499E-04   1.47572E+02
CO2(aq)                             CO2(aq)   3.86103E-04   1.12115E-03   2.904         3.86106E-04   3.45643E-04   1.52117E+01
HCO3-                                  HCO3-  2.26571E-04   8.38810E-05   0.3702        2.26573E-04   2.02829E-04   1.23760E+01    1.23E-14
H+                                     H+     1.21872E-06   4.78095E-06   3.923         1.21872E-06   1.09101E-06   1.09962E-03    1.23E-14
NpO2CO3-                            NpO2CO3-  1.33526E-07   2.42971E-07   1.820         1.33527E-07   1.19534E-07   3.93334E-02    1.85E-14
CO3=                                   CO3=   3.09384E-08   8.03343E-10   2.5966E-02    3.09386E-08   2.76963E-08   1.66203E-03    0.00E+00
OH-                                    OH-    3.01685E-09   1.61977E-09   0.5435        3.01687E-09   2.70071E-09   4.59318E-05    1.23E-14
NpO2OH(aq)                          NpO2OH(aq)   7.72186E-10   7.72186E-10   1.000         7.72191E-10   6.91267E-10   1.97740E-04   -6.17E-15
NpO2(CO3)2=-                        NpO2(CO3)2=-  1.98384E-11   5.13355E-16   2.5877E-05    1.98385E-11   1.77595E-11   6.90960E-06    0.00E+00
NpO2(OH)2-                          NpO2(OH)2-    2.04381E-16   6.10703E-17   0.2988        2.04383E-16   1.82964E-16   5.54494E-11    0.00E+00
NpO2(CO3)3=--                       NpO2(CO3)3=-- 1.25197E-16   9.87897E-26   7.8908E-10    1.25198E-16   1.12077E-16   5.03310E-11   -3.25E-09
HCl(aq).....to.titrate.acid.only               0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
NaOH(aq).....to.titrate.base.only              0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.99E+02
NpO2OH(amor)_____________NpO2OH(amor)          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
Na3H(CO3)2.2H2O_____________Trona              0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
Na2CO3.H2O_____Thermonatrite                   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.10H2O_____________Natron                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
NaHCO3_____________Nahcolite                   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
NaCl_____________Halite                        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NpO2OH(aged)_____________NpO2OH(aged)          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
pH (-log[aH+]); pmH(-log[mH+])      5.3205      5.9141
Osmotic Coefficient=    1.241871
Equilibrium RH (%) =   77.795863
Ionic Strength (m) =    5.611188
Density, kg/m3     =    1188.93
fCO2(g); log[fCO2(g)]=                                  3.400E-02    -1.47

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -1.33323084E+04
Flushing Titration #            1
# inversions for batch pblm           17
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.85857174E+01    1.11017591E+02   9.93838868E+01   1.00169020E+05  Hydrogen
  3.66707638E+01    5.55113597E+01   4.96942389E+01   7.95078006E+05  Oxygen
  5.42543623E+00    5.61057382E+00   5.02263316E+00   1.15469181E+05  Sodium
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95016801E+00    5.61096098E+00   5.02297975E+00   1.78079701E+05  Chlorine
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  1.47561578E+00    6.12839260E-04   5.48618892E-04   6.58946151E+00  Carbon
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Fe(II)
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Mg(II)
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Tracer(I)
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  1.47561578E+00    6.12839260E-04   5.48618892E-04   1.30049121E+02  Np(V)
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00    0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.94659251E-15   -5.60067366E-15  -5.01377045E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      461.602144251003      grams
    H2O MASS           347.563995068949      grams
    TDS(g/kg)          328.106912108174      g/kgH2O

  Specified Solution Density
    DENSITY            1188.93254605458      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.388249228926239       liters
    TDS              293.724084133903        g/l

  Density based on TDS and NaCl solutions    1188.93254605458      g/l
  Percent relative error vs NaCl density     0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                              WATER        8.31822E-01   7.77959E-01   0.9352        1.92928E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)        9.99932E+00   1.00000E+00   1.000         3.47540E+00   8.95147E+00   3.15133E+06
Cl-                              Cl-          5.61096E+00   5.29329E+00   0.9434        1.95017E+00   5.02298E+00   1.78080E+05
Na+                              Na+          5.61057E+00   5.29268E+00   0.9433        1.95003E+00   5.02263E+00   1.15469E+05
NpO2+                            NpO2+        6.12705E-04   1.21978E-03   1.991         2.12954E-04   5.48499E-04   1.47572E+02
CO2(aq)                          CO2(aq)      3.86103E-04   1.12115E-03   2.904         1.34196E-04   3.45643E-04   1.52117E+01
HCO1-                            HCO3-        2.26571E-04   8.38810E-05   0.3702        7.87481E-05   2.02829E-04   1.23760E+01   -5.15E-12
H+                               H+           1.21872E-06   4.78095E-06   3.923         4.23582E-07   1.09101E-06   1.09962E-03   -2.29E-11
NpO2CO3-                         NpO2CO3-     1.33526E-07   2.42971E-07   1.820         4.64090E-08   1.19534E-07   3.93334E-02    1.85E-14
CO3=                             CO3=         3.09384E-08   8.03343E-10   2.5966E-02    1.07531E-08   2.76963E-08   1.66203E-03    1.68E-11
OH-                              OH-          3.01685E-09   1.63977E-09   0.5435        1.04855E-09   2.70071E-09   4.59318E-05    2.30E-11
NpO2OH(aq)                       NpO2OH(aq)   7.72186E-10   7.72186E-10   1.000         2.68384E-10   6.91267E-10   1.97740E-04    6.15E-12
NpO2(CO3)2=-                     NpO2(CO3)2=- 1.98384E-11   5.11355E-16   2.5877E-05    6.89511E-12   1.77595E-11   6.90960E-06    1.69E-11
NpO2(OH)2-                       NpO2(OH)2-   2.04381E-16   6.10703E-17   0.2988        7.10356E-17   1.82964E-16   5.54494E-11    2.92E-11
NpO2(CO3)3===-                   NpO2(CO3)3===- 1.35197E-16  9.87897E-26   7.8908E-10    4.35139E-17   1.12077E-16   5.03110E-11   -3.15E-10
HCl(aq).....to.titrate.acid.only              0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
NaOH(aq).....to.titrate.base.only             0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.99E+02
Na3H(CO3)2.2H2O_____________Trona             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
Na2CO3.H2O_____Thermonatrite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.10H2O_____________Natron               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
NaHCO3_____________Nahcolite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
NaCl_____________Halite                       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NpO2OH(amor)_____________NpO2OH(amor)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
NpO2OH(aged)_____________NpO2OH(aged)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00

pH (-log[aH+]); pmH(-log[mH+])      5.3205      5.9141
Osmotic Coefficient=    1.241871
Equilibrium RH (%) =   77.795863
Ionic Strength (m) =    5.611188
Density, kg/m3     =    1188.93
fCO2(g); log[fCO2(g)]=                                  3.400E-02    -1.47

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -4.63379813E+03
Flushing Titration #            2
# inversions for batch pblm           19
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
611
612  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter
613
614  3.85957275E+01  1.11017746E+02  9.93891116E+01  1.00174286E+05  Hydrogen
615  3.66763098E+01  5.55107903E+01  4.96962723E+01  7.95110540E+04  Oxygen
616  5.42594206E+00  5.61014105E+00  5.02250276E+00  1.15466183E+05  Sodium
617  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
618  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
619  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
620  1.95031318E+00  5.60993114E+00  5.02231483E+00  1.78056128E+05  Chlorine
621  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
622  3.47579611E+00  6.90932337E-04  6.18560128E-04  7.42952570E+00  Carbon
623  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  PosIon
624  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  NegIon
625  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
626  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
627  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
628  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
629  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Th(IV)
630  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
631  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
632  3.47561578E+00  1.72218651E-04  1.54179484E-04  3.65479691E+01  Np(V)
633  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  ClO4-(EL)
634  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
635  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electron
636 -1.36380199E-15 -3.92287521E-15 -3.51197080E-15  0.00000000E+00  Charge
637
638  Solution Parameters, Calculated
639    SOLUTION MASS      461.665999617212      grams
640    H2O MASS           347.653675849709      grams
641    TDS(g/kg)          327.947988724245      g/kgH2O
642
643  Specified Solution Density
644    DENSITY            1188.85111378691      kg/m^3 = g/l
645
646  Solution Parameters Based on Specified Density
647    SOLUTION VOL     0.388329534508861       liters
648    TDS              293.596838859294        g/l
649
650  Density based on TDS and NaCl solutions     1188.85111378691      g/l
651  Percent relative error vs NaCl density    0.000000000000000E+000 %
652
653
654
655  TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
656
657  Species Name                          Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
658
659  H2O                          WATER    8.31845E-01   7.78011E-01   0.9353        1.92978E+01   6.96944E+01   8.95254E+05
660  NaNpO2CO3(s)_____NaNpO2CO3(s)         9.99710E+00   1.00000E+00   1.000         3.47556E+00   8.95002E+00   3.15082E+06
661  Na+                           Na+     5.61014E+00   5.29140E+00   0.9432        1.95039E+00   5.02250E+00   1.15466E+05
662  Cl-                           Cl-     5.60993E+00   5.29139E+00   0.9432        1.95031E+00   5.02231E+00   1.78056E+05
663  HCO3-                         HCO3-   3.82212E-04   1.41513E-04   0.3702        1.32878E-04   3.42177E-04   2.08787E+01
664  CO2(aq)                       CO2(aq) 3.08476E-04   8.95671E-04   2.904         1.07243E-04   2.76165E-04   1.21539E+01
665  NpO2+                         NpO2+   1.72085E-04   3.42681E-04   1.990         5.98258E-05   1.54059E-04   4.14492E+01  -1.82E-10
666  H+                            H+      5.77346E-07   2.26410E-06   3.922         2.00716E-07   5.16872E-07   5.20955E-04  -2.18E-10
667  NpO2CO3-                      NpO2CO3- 1.33573E-07  2.43030E-07   1.819         4.64370E-08   1.19561E-07   3.93490E-02   8.02E-14
668  CO3=                          CO3=    1.10196E-07   2.86188E-09   2.5971E-02    3.83099E-08   9.86531E-08   5.92010E-03   3.31E-10
669  OH-                           OH-     6.37029E-09   3.46282E-09   0.5436        2.21466E-09   5.70303E-09   9.69932E-05   2.19E-10
670  NpO2OH(aq)                    NpO2OH(aq) 4.57851E-10  4.57851E-10  1.000        1.59174E-10   4.09893E-10   1.17252E-04  -1.14E-10
671  NpO2(CO3)2=-                  NpO2(CO3)2=- 7.06677E-11  1.82925E-15  2.5885E-05  2.45679E-11  6.32656E-11  2.46164E-05   3.32E-10
672  NpO2(CO3)3=5-                 NpO2(CO3)3=5- 1.58546E-15  1.25406E-24  7.9097E-10  5.51192E-16  1.41939E-15  6.37413E-10   5.26E-10
673  NpO2(OH)2-                    NpO2(OH)2-  2.55903E-16  7.64679E-17  0.2988        8.89657E-17  2.29098E-16  6.94309E-11   1.05E-10
674  HCl(aq).....to.titrate.acid.only      0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
675  NaOH(aq).....to.titrate.base.only     0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+02
676  NpO2OH(aged)_____NpO2OH(aged)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.61E+00
677  NpO2OH(amor)_____NpO2OH(amor)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.21E+00
678  NaJNpO2(CO3)2(s)_DISABLED_DISABLED    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
679  NaCl_____Halite                       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
680  NaHCO3_____Nahcolite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.72E+00
681  Na2CO3.10H2O_____Natron               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.36E+00
682  Na2CO3.7H2O____Na2CO3-Heptahydrate    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.40E+00
683  Na2CO3.H2O_____Thermonatrite          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.69E+00
684  NaJH(CO3)2.2H2O_____Trona             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.40E+00
685
686  pH (-log[aH+]); pmH(-log[mH+])      5.6451        6.2386
687  Osmotic Coefficient=    1.241740
688  Equilibrium RH (%) =   77.801108
689  Ionic Strength (m) =    5.610314
690  Density, kg/m3     =    1188.85
691  fCO2(g); log[fCO2(g)]=                                  2.716E-02     -1.57
692
693  NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
694          - Gas "molality" and "activity" are gas partial pressures
695          - "Descriptor" means:
696            "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
697            "Saturation Index for minerals, SI=log10(IAP/Ksp)
698            "log10(activity) for aqueous species with very small concentrations
699            "log10(partial pressure) for gases
700
701  Total G/RT=    -4.634380311E+03
702  Flashing Titration #          3
703  # inversions for batch pblm          28
704 1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.6lmolal NaCl   FMT V2.3
705  DATABASE:  NEW84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
706  95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,PRF90,P91,RFFR92,RFF94,RRFP94)
707      Pressure=      1.00000E+00 (=) ATM      Temperature=      2.98E+02 [=] Kelvin
708
709  Elemental Abundances for Flash Problem
710
711    Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter
712
713    3.85999827E+01  1.11017943E+02  9.93906557E+01  1.00175842E+05  Hydrogen
714    3.66786675E+01  5.55109442E+01  4.96970938E+01  7.95123682E+04  Oxygen
715    5.42615710E+00  5.61002979E+00  5.02247225E+00  1.15465482E+05  Sodium
716    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
717    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
718    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
719    1.95037489E+00  5.60950015E+00  5.02199808E+00  1.78044898E+05  Chlorine
720    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
721    3.47587277E+00  7.90126088E-04  7.07373490E-04  8.49626299E+00  Carbon
722    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  PosIon
723    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  NegIon
724    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
725    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
726    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
727    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
728    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Th(IV)
729    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
730    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
731    3.47561578E+00  5.09860840E-05  4.56460696E-05  1.08203186E+01  Np(V)
732    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  ClO4-(EL)
733    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
734    0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electron
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
 -2.11316242E-15  -6.07769560E-15  -5.44115783E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      461.701224245767        grams
    H2O MASS           347.691387660714        grams
    TDS(g/kg)          327.905264930827        g/kgH2O

  Specified Solution Density
    DENSITY            1188.82922071360        kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.388366315532375         liters
    TDS              293.562628954490          g/l

  Density based on TDS and NaCl solutions     1188.82922071360      g/l
  Percent relative error vs NaCl density     0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                WATER      8.31852E-01   7.78030E-01   0.9353        1.92999E+01   4.96951E+01   8.95267E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)        9.99622E+00   1.00000E+00   1.000         3.47560E+00   8.94928E+00   3.15056E+06
Na+                                Na+        5.61003E+00   5.29080E+00   0.9431        1.95056E+00   5.02247E+00   1.15465E+05
Cl-                                Cl-        5.60950E+00   5.29073E+00   0.9432        1.95057E+00   5.02200E+00   1.78045E+05
HCO3-                              HCO3-      5.79856E-04   2.14695E-04   0.3703        2.01611E-04   5.19125E-04   1.16755E+01
CO2(aq)                            CO2(aq)    2.09763E-04   6.09044E-04   2.903         7.29329E-05   1.87794E-04   8.26478E+00
NpO2+                              NpO2+      5.08519E-05   1.01191E-04   1.990         1.76808E-05   4.55260E-05   1.22486E+01   -1.63E-10
CO3=                               CO3=       3.72979E-07   9.68710E-09   2.5972E-02    1.29682E-07   3.33916E-07   2.00380E-02    1.16E-10
H+                                 H+         2.58813E-07   1.01480E-06   3.921         8.99871E-08   2.31707E-07   2.33537E-04   -1.00E-10
NpO2CO3-                           NpO2CO3-   1.33591E-07   2.43057E-07   1.819         4.64484E-08   1.19600E-07   3.93550E-02    3.70E-14
OH-                                OH-        1.42123E-08   7.72603E-09   0.5436        4.94149E-09   1.27238E-08   2.16397E-04    1.02E-10
NpO2OH(aq)                         NpO2OH(aq) 3.01826E-10   3.01826E-10   1.000         1.04942E-10   2.70215E-10   7.72962E-05   -2.15E-11
NpO2(CO3)2=-                       NpO2(CO3)2=- 2.39201E-10  6.19248E-15   2.5888E-05    8.31683E-11   2.14149E-10   8.33180E-05    1.24E-10
NpO2(CO3)3=-                       NpO2(CO3)3=- 1.81540E-14  1.43698E-23   7.9155E-10    6.31199E-15   1.62527E-14   7.29866E-09   -3.61E-07
NpO2(OH)2-                         NpO2(OH)2- 3.76383E-16    1.12471E-16   0.2988        1.30865E-16   3.36963E-16   1.02121E-10    8.05E-11
HCl(aq).....to.titrate.acid.only              0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
NaOH(aq).....to.titrate.base.only             0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+02
NpO2OH(aged)_____________NpO2OH(aged)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.79E+00
NpO2OH(amor)_____________NpO2OH(amor)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.39E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.35E+02
NaCl_____________________Halite               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3___________________Nahcolite            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.54E+00
Na2CO3.10H2O_____________Natron               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -6.83E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -6.87E+00
Na2CO3.H2O_____________Thermonatrite          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.16E+00
Na3H(CO3)2.2H2O_____________Trona             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.68E+00

pH (-log(aH+)), pmH(-log[mH+])       5.9936       6.5870
Osmotic Coefficient=    1.241681
Equilibrium RH (%) =   77.803013
Ionic Strength (m) =    5.610081
Density, kg/m3     =    1188.83
fCO2(g), log[fCO2(g)]=                                    1.847E-02    -1.73

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -4.63462770E+03
Flashing Titration #        4
# inversions for batch phin          20
1Benchmark TITRUE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
 DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (KR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 (=) ATM     Temperature=     2.98E+02 (=) Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.86060470E+01   1.11018357E+02   9.93915462E+01   1.00176739E+05  Hydrogen
  3.66820273E+01   5.55118409E+01   4.96981566E+01   7.95140687E+05  Oxygen
  5.42646354E+00   5.61000023E+00   5.02247206E+00   1.15465478E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95046284E+00   5.60889282E+00   5.02148063E+00   1.78026553E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47598202E+00   1.95369170E-03   9.41341702E-04   1.11304772E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   5.04731448E-07   4.51871568E-07   1.07115342E-01  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.15000139E-15  -3.30702765E-15  -2.96068686E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      461.766388131807        grams
    H2O MASS           347.744715353108        grams
    TDS(g/kg)          327.889016696973        g/kgH2O

  Specified Solution Density
    DENSITY            1188.82089442743        kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.388423849459851         liters
    TDS              293.549616380179          g/l

  Density based on TDS and NaCl solutions     1188.82089442743      g/l
  Percent relative error vs NaCl density     0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                WATER      8.31857E-01   7.78050E-01   0.9353        1.93039E+01   4.96953E+01   8.95271E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)        9.99473E+00   1.00000E+00   1.000         3.47562E+00   8.94800E+00   3.15011E+06
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

Na+	Na+	5.61000E+00	5.29000E+00	0.9430	1.95085E+00	5.02247E+00	1.15465E+05	
Cl-	Cl-	5.60889E+00	5.28999E+00	0.9431	1.95046E+00	5.02148E+00	1.78027E+05	
HCO3-	HCO3-	9.92660E-04	1.67543E-04	0.3703	3.45192E-04	8.88700E-04	5.42259E+01	
CO3=	CO3=	5.67888E-05	1.47494E-06	2.5972E-02	1.97480E-05	5.08414E-05	3.05095E+00	
CO2(aq)	CO2(aq)	4.03765E-06	1.17227E-05	2.903	1.40400E-06	3.61461E-06	1.59078E-01	-4.22E-08
OH-	OH-	1.26397E-06	6.87170E-07	0.5437	4.39540E-07	1.13160E-06	1.92454E-02	-9.05E-08
NpO2+	NpO2+	3.34101E-07	6.64703E-07	1.990	1.16182E-07	2.99111E-07	8.04750E-02	1.77E-07
NpO2CO3-	NpO2CO3-	1.33613E-07	2.43094E-07	1.819	4.64631E-08	1.19620E-07	3.93616E-02	3.70E-13
NpO2(CO3)2=	NpO2(CO3)2=	3.64205E-08	9.43001E-13	2.5892E-05	1.26650E-08	3.26062E-08	1.26859E-02	-1.13E-07
N+	N+	2.91065E-09	1.14100E-08	3.920	1.01216E-09	2.60582E-09	2.62641E-06	1.24E-07
NpO2(CO3)3==	NpO2(CO3)3==	4.20660E-10	3.33181E-19	7.9204E-10	1.46282E-10	3.76605E-10	1.69124E-04	-2.13E-07
NpO2OH(aq)	NpO2OH(aq)	1.76339E-10	1.76339E-10	1.000	6.13211E-11	1.57872E-10	4.51598E-05	-2.03E-08
NpO2(OH)2-	NpO2(OH)2-	1.95583E-14	5.84438E-15	0.2988	6.80128E-15	1.75100E-14	5.30660E-09	-1.48E-07
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.47E+02
NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.96E+02
NpO2OH(aged)_____NpO2OH(aged)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.01E+00
NpO2OH(amor)_____NpO2OH(amor)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.62E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.33E+02
NaCl_____Halite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
NaHCO3_____Nahcolite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.31E+00
Na2CO3.10H2O_____Natron		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.65E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.69E+00
Na2CO3.H2O_____Thermonatrite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.98E+00
Na3H(CO3)2.2H2O_____Trona		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.27E+00

pH (-log[aH+]); pmH(-log[mH+]) 7.9427 8.5360
Osmotic Coefficient= 1.241601
Equilibrium RH (%) = 77.805007
Ionic Strength (m) = 5.610057
Density, kg/m3 = 1188.82
fCO2(g); log[fCO2(g)]= 3.555E-04 -3.45

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
"dG/RT/ln10 for species with nontero concs. (convergence criterion)
"Saturation Index for minerals, SI=log10(IAP/Ksp)
"log10(activity) for aqueous species with very small concentrations
"log10(partial pressure) for gases

Total G/RT= -6.61497997E+03
Flashing Titration # 5
inversions for batch pblm 22

1Benchmark TITRATE Problem. LOG10 option; Np(V)O2 with CO3 in 5.6lmolal NaCl FMT V2.3
DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (HW94);
95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFP94,RRFP94)
Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.86146891E+01	1.11018383E+02	9.93917155E+01	1.00176910E+05	Hydrogen
3.66868155E+01	5.55131961E+01	4.96994430E+01	7.95161268E+05	Oxygen
5.42690025E+00	5.61000156E+00	5.02248064E+00	1.15465675E+05	Sodium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1.95058817E+00	5.60799916E+00	5.02068795E+00	1.77998450E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47613771E+00	1.50108527E-03	1.34388050E-03	1.61413487E+01	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
3.47561578E+00	5.18420811E-07	4.64127943E-07	1.10020691E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Cl04-(EL)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
-1.62616037E-15	-4.67525956E-15	-4.18563175E-15	0.00000000E+00	Charge

Solution Parameters, Calculated
SOLUTION MASS 461.868060856166 grams
H2O MASS 347.822478666644 grams
TDS(g/kg) 327.884450213538 g/kgH2O

Specified Solution Density
DENSITY 1188.61855435140 kg/m^3 = g/l

Solution Parameters Based on Specified Density
SOLUTION VOL 0.388510138208732 liters
TDS 293.545961799973 g/l

Density based on TDS and NaCl solutions 1188.61855435140 g/l
Percent relative error vs NaCl density 0.000000000000000E+000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31862E-01	7.78867E-01	0.9353	1.93072E+01	4.96954E+01	8.95273E+05	
NaNpO2CO3(s)_____NaNpO2CO3(s)		9.99250E+00	1.00000E+00	1.000	3.47562E+00	8.94601E+00	3.14941E+06	
Na+	Na+	5.61000E+00	5.28971E+00	0.9429	1.95128E+00	5.02248E+00	1.15466E+05	
Cl-	Cl-	5.60800E+00	5.28867E+00	0.9431	1.95059E+00	5.02069E+00	1.77998E+05	
HCO3-	HCO3-	1.00903E-03	1.73572E-04	0.1702	3.50963E-04	9.03356E-04	5.51202E+01	
CO3=	CO3=	4.90717E-04	1.27445E-05	2.5971E-02	1.70682E-04	4.39325E-04	2.63636E+01	
OH-	OH-	1.07447E-05	5.84190E-06	0.5437	3.73726E-06	9.61946E-06	1.63601E-01	-6.54E-08
CO2(aq)	CO2(aq)	4.82702E-07	1.40153E-06	2.904	1.67895E-07	4.32150E-07	1.90188E-02	-8.59E-08
NpO2(CO3)2=	NpO2(CO3)2=	3.14571E-07	8.14859E-12	2.5904E-05	1.09415E-07	2.81627E-07	1.09571E-01	2.57E-08
NpO2CO3-	NpO2CO3-	1.33630E-07	2.43107E-07	1.819	4.64794E-08	1.19635E-07	3.93666E-02	4.47E-12
NpO2+	NpO2+	3.86807E-08	7.69314E-08	1.989	1.34540E-08	3.46298E-08	9.31704E-03	-2.12E-08
NpO2(CO3)3==	NpO2(CO3)3==	3.13656E-08	2.48770E-17	7.9313E-10	1.09097E-08	2.80808E-08	1.26104E-02	4.46E-08
H+	H+	3.42512E-10	1.34216E-09	3.919	1.19134E-10	3.06642E-10	3.09064E-07	-2.53E-08
NpO2OH(aq)	NpO2OH(aq)	1.73507E-10	1.73507E-10	1.000	6.03495E-11	1.55336E-10	4.44344E-05	4.67E-09
NpO2(OH)2-	NpO2(OH)2-	1.63614E-13	4.88873E-14	0.2988	5.69085E-14	1.46479E-13	4.43921E-08	2.97E-08
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
NpO2OH(aged)_____NpO2OH(aged)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.01E+00
NpO2OH(amor)_____NpO2OH(amor)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.61E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.32E+02
NaCl_____Halite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
NaHCO3_____Nahcolite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+00
Na2CO3.10H2O_____Natron		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.71E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.75E+00
Na2CO3.H2O_____Thermonatrite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.04E+00
Na3H(CO3)2.2H2O_____Trona		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.33E+00

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
pH (-log[aH+]); pmH(-log[mH+])      8.8722      9.4653
Osmotic Coefficient=    1.241539
Equilibrium RH (%) =   77.806749
Ionic Strength (m) =    5.610494
Density, kg/m3     =    1188.82
fCO2(g); log[fCO2(g)]=                                  4.250E-05    -4.37

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.63548129E+03
Flushing Titration #        6
# inversions for batch pblm          23
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  MMH84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR85,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM      Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

  3.86270051E+01    1.11018410E+02    9.93919460E+01    1.00177142E+05  Hydrogen
  1.66936391E+01    5.55151239E+01    4.97012721E+01    7.95190533E+05  Oxygen
  5.42752260E+00    5.61000344E+00    5.02249276E+00    1.15465953E+05  Sodium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
  1.95076678E+00    5.60672579E+00    5.01955836E+00    1.77958403E+05  Chlorine
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
  3.47635958E+00    2.13880634E-03    1.91481868E-03    2.29988871E-01  Carbon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  PosIon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  NegIon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Th(IV)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
  3.47561578E+00    1.02583551E-06    9.18404325E-07    2.17706092E-01  Np(V)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
 -1.31308874E-15   -3.77396651E-15   -3.37873581E-15    0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      462.013014691330      grams
    H2O MASS           347.933330560296      grams
    TDS(g/kg)          327.877998698106      g/kgH2O

  Specified Solution Density
    DENSITY            1188.81524828657      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388633149984595        liters
    TDS             293.540795775029         g/l

  Density based on TDS and NaCl solutions     1188.81524828657      g/l
  Percent relative error vs NaCl density     0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles    Molarity      mg/liter      Descriptor

H2O                                  WATER  8.31870E-01   7.78092E-01   0.9354       1.93133E+01   4.96955E+01   8.95274E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.98931E+00   1.00000E+00    1.000       3.47562E+00   8.94318E+00   3.14841E+06
Na+                                  Na+   5.61000E+00   5.28932E+00   0.9428       1.95191E+00   5.02249E+00   1.15466E+05
Cl-                                  Cl-   5.60673E+00   5.28679E+00   0.9429       1.95077E+00   5.01956E+00   1.77958E+05
CO3=                                 CO3=  1.11398E-03   2.89293E-05   2.5969E-02   3.87591E-04   9.97318E-04   5.98462E+01
HCO3-                                HCO3- 1.02256E-01   3.76536E-04   0.3702       3.55784E-04   9.15475E-04   5.58596E+01
OH-                                  OH-   2.40684E-05   1.30873E-05   0.5438       8.37419E-06   2.15478E-05   3.66470E-01   -4.77E-09
NpO2(CO3)2=-                  NpO2(CO3)2=-  7.13649E-07   1.84983E-11   2.5921E-05   2.48302E-07   6.38912E-07   2.48578E-01    9.86E-09
CO2(aq)                              CO2(aq) 2.18328E-07   6.33927E-07    2.904       7.59637E-08   1.95464E-07   8.60232E-03   -3.55E-08
NpO2(CO3)3=5-                 NpO2(CO3)3=5- 1.61312E-07   1.28193E-16   7.9469E-10   5.61257E-08   1.44418E-07   6.48546E-02    1.95E-08
NpO2CO3-                          NpO2CO3-  1.33654E-07   2.43125E-07    1.819       4.65026E-08   1.19657E-07   3.93738E-02    1.56E-12
NpO2+                                NpO2+  1.70494E-08   3.38938E-08    1.988       5.93207E-09   1.52639E-08   4.10671E-03   -9.06E-09
NpO2OH(aq)                      NpO2OH(aq)  1.71249E-10   1.71249E-10    1.000       5.95833E-11   1.53315E-10   4.38564E-05    1.05E-08
H+                                   H+    1.52979E-10   5.99129E-10    3.916       5.32265E-11   1.36950E-10   1.38040E-07   -1.95E-08
NpO2(OH)2-                    NpO2(OH)2-    3.61806E-13   1.08095E-13   0.2988       1.25884E-13   3.23915E-13   9.81663E-08    3.00E-08
HCl(aq).....to.titrate.acid.only           0.00000E+00   0.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
NaOH(aq).....to.titrate.base.only          0.00000E+00   0.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+02
NpO2OH(aged)_____________NpO2OH(aged)      0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.04E+00
NpO2OH(amor)_____________NpO2OH(amor)      0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.63E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED         0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -9.32E+02
NaCl_____________________________Halite    0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
NaHCO3___________________________Nahcolite 0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.30E+00
Na2CO3.10H2O_____________________Natron    0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.36E+00
Na2CO3.7H2O____Na2CO3-HeptAhydrate         0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.39E+00
Na2CO3.H2O_____________Thermonatrite       0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.68E+00
Na3H(CO3)2.2H2O_____________Trona          0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -4.96E+00

pH (-log[aH+]); pmH(-log[mH+])      9.2225      9.8154
Osmotic Coefficient=    1.241451
Equilibrium RH (%) =   77.809237
Ionic Strength (m) =    5.611121
Density, kg/m3     =    1188.82
fCO2(g); log[fCO2(g)]=                                  1.922E-05    -4.72

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.63619544E+03
Flushing Titration #        7
# inversions for batch pblm          23
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  MMH84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM      Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.86445565E+01	1.11018446E+02	9.93922712E+01	1.00177470E+05	Hydrogen
3.67033634E+01	5.55178692E+01	4.97038762E+01	7.95232197E+05	Oxygen
5.42840953E+00	5.61000623E+00	5.02251004E+00	1.15466351E+05	Sodium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1.95102131E+00	5.60491242E+00	5.01794965E+00	1.77901369E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47667578E+00	3.04711826E-03	2.72801516E-03	3.27661900E+01	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
3.47561578E+00	1.94421849E-06	1.74061427E-06	4.12609479E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Cl04-(EL)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
-2.12321556E-15	-6.09959368E-15	-5.46082646E-15	0.00000000E+00	Charge

Solution Parameters, Calculated

SOLUTION MASS	462.219612785907	grams
H2O MASS	348.091311120332	grams
TDS(g/kg)	327.868860898173	g/kgH2O

Specified Solution Density

DENSITY	1188.81056561769	kg/m^3 = g/l

Solution Paramaters Based on Specified Density

SOLUTION VOL	0.388808466339415	liters
TDS	293.533478681879	g/l

Density based on TDS and NaCl solutions 1188.81056561769 g/l
Percent relative error vs NaCl density 0.000000000000000E+000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31881E-01	7.78127E-01	0.9354	1.93221E+01	4.96957E+01	8.95277E+05	
NaNpO2CO3(s)	NaNpO2CO3(s)	9.98478E+00	1.00000E+00	1.000	3.47562E+00	8.93914E+00	3.14699E+06	
Na+	Na+	5.61001E+00	5.28876E+00	0.9427	1.95279E+00	5.02251E+00	1.15466E+05	
Cl-	Cl-	5.60491E+00	5.28411E+00	0.9428	1.95102E+00	5.01795E+00	1.77901E+05	
CO3=	CO3=	2.00201E-03	5.19857E-05	2.5967E-02	6.96883E-04	1.79236E-03	1.07558E+02	
HCO3-	HCO3-	1.04073E-03	3.85192E-04	0.3701	3.62268E-04	9.31738E-04	5.68519E+01	
OH-	OH-	4.24988E-05	2.31125E-05	0.5438	1.47935E-05	3.80482E-05	6.47098E-01	-6.11E-08
NpO2(CO3)2=-	NpO2(CO3)2=-	1.28137E-06	3.32447E-11	2.5945E-05	4.46032E-07	1.14718E-06	4.46327E-01	4.76E-08
NpO2(CO3)3=3-	NpO2(CO3)3=3-	5.19502E-07	4.13999E-16	7.9692E-10	1.80834E-07	4.65098E-07	2.08864E-01	1.05E-07
NpO2CO3-	NpO2CO3-	1.33688E-07	2.43151E-07	1.819	4.65356E-08	1.19688E-07	3.93840E-02	1.15E-12
CO2(aq)	CO2(aq)	1.25799E-07	3.65269E-07	2.904	4.37894E-08	1.12625E-07	4.95659E-03	-3.36E-07
NpO2+	NpO2+	9.49498E-09	1.88634E-08	1.987	3.30512E-09	8.50064E-09	2.28707E-03	-4.00E-08
NpO2OH(aq)	NpO2OH(aq)	1.68316E-10	1.68316E-10	1.000	5.85892E-11	1.50689E-10	4.31052E-05	1.03E-07
H+	H+	8.66954E-11	3.39269E-10	3.913	1.01779E-11	7.76164E-11	7.82296E-08	-1.46E-07
NpO2(OH)2-	NpO2(OH)2-	6.28105E-13	1.87627E-13	0.2987	2.18638E-13	5.62228E-13	1.70420E-07	2.42E-07
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.49E+02
NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.94E+02
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.05E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.64E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.31E+02
NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.29E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.10E+00
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.14E+00
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.43E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.70E+00

pH (-log[aH+]); pmH(-log[mH+]) 9.4695 10.0620
Osmotic Coefficient= 1.241325
Equilibrium RH (%) = 77.812731
Ionic Strength (m) = 5.612017
Density, kg/ml = 1188.81
fCO2(g); log[fCO2(g)]= 1.108E-05 -4.96

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -4.63721298E+03
Flashing Titration # 8
inversions for batch pblm 29
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
DATABASE: NMM84/FM86; Np(V)-Na-CO3-OH-Cl-Cl04 (NR94);
95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,PRP90,P91,RFPR92,RTF94,RUFP94)
Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.86695692E+01	1.11018496E+02	9.93927291E+01	1.00177932E+05	Hydrogen
3.67172215E+01	5.55217779E+01	4.97075822E+01	7.95291491E+05	Oxygen
5.42967348E+00	5.61001045E+00	5.02253469E+00	1.15466917E+05	Sodium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1.95138405E+00	5.60233091E+00	5.01565935E+00	1.77820171E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47712639E+00	4.34048558E-03	3.88595344E-03	4.66741868E+01	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
3.47561578E+00	3.60501967E-06	3.22750493E-06	7.65074233E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Cl04-(EL)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
-1.20892820E-15	-3.47077543E-15	-3.10731863E-15	0.00000000E+00	Charge

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  Solution Parameters, Calculated
    SOLUTION MASS      462.514079623503      grams
    H2O MASS           348.316456438661      grams
    TDS(g/kg)          327.855951316366      g/kgH2O

  Specified Solution Density
    DENSITY            1188.80395005085      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.389058330100366       liters
    TDS                293.523141261063      g/l

  Density based on TDS and NaCl solutions     1188.80395005085      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                          Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                          WATER    8.31897E-01   7.78177E-01   0.9354        1.93346E+01   4.96959E+01   8.95281E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s) 9.97832E+00   1.00000E+00    1.000        3.47561E+00   8.93340E+00   3.14497E+06
Na+                           Na+     5.61001E+00   5.28798E+00   0.9426        1.95406E+00   5.02253E+00   1.15467E+05
Cl-                           Cl-     5.60233E+00   5.28028E+00   0.9425        1.95138E+00   5.01566E+00   1.77820E+05
CO3=                          CO3=    3.26656E-03   8.48095E-05   2.5963E-02    1.13780E-03   2.92449E-03   1.75496E+02
HCO3-                         HCO3-   1.06541E-03   3.94227E-04   0.3700        3.71098E-04   9.53837E-04   5.82004E+01
OH-                           OH-     6.77337E-05   1.68439E-05   0.5440        2.35928E-05   6.06407E-05   1.03133E+00   -3.39E-10
NpO2(CO3)2=-          NpO2(CO3)2=-    2.08796E-06   5.42434E-11   2.5979E-05    7.27272E-07   1.86931E-06   7.27266E-01    2.35E-09
NpO2(CO3)3=5-      NpO2(CO3)3=5-      1.37733E-06   1.10201E-15   8.0011E-10    4.79745E-07   1.23309E-06   5.53751E-01    4.83E-09
NpO2CO3-                NpO2CO3-     1.33737E-07   2.43187E-07    1.818        4.65827E-08   1.19732E-07   3.93986E-02    1.22E-12
CO2(aq)                 CO2(aq)      8.07635E-08   2.34511E-07   2.904         2.81313E-08   7.23060E-08   3.18217E-03   -1.77E-08
NpO2+                   NpO2+        5.82643E-09   1.15644E-08   1.985         2.02944E-09   5.21629E-09   1.40343E-03   -2.32E-09
NpO2OH(aq)              NpO2OH(aq)   1.64493E-10   1.64493E-10   1.000         5.72955E-11   1.47267E-10   4.21264E-05    7.48E-09
H+                            H+     5.44489E-11   2.12840E-10   3.909         1.89655E-11   4.87471E-11   4.91322E-08   -9.80E-09
NpO2(OH)2-              NpO2(OH)2-   9.78743E-13   2.92306E-13   0.2987        3.40912E-13   8.76250E-13   2.65558E-07    1.73E-08
HCl(aq).....to.titrate.acid.only     0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
NaOH(aq)....to.titrate.base.only     0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
NpO2OH(aged)_____________NpO2OH(aged) 0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.06E+00
NpO2OH(amor)_____________NpO2OH(amor) 0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.65E+00
Na3Np02(CO3)2(s)_DISABLED_DISABLED    0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+02
NaCl_____________________Halite       0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
NaHCO3___________________Nahcolite    0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.28E+00
Na2CO3.10H2O_____Natron               0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.89E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate    0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.93E+00
Na2CO3.H2O_________Thermonatrite      0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.22E+00
Na3H(CO3)2.2H2O_____________Trona     0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.48E+00

pH (-log[aH+]); pmH(-log[mH+])        9.6719       10.2640
Osmotic Coefficient=    1.241147
Equilibrium RH (%) =   77.817733
Ionic Strength (m) =    5.613297
Density, kg/m3     =    1188.80
fCO2(g); log[fCO2(g)]=                                 7.112E-06    -5.15

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Kep)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -4.63866284E+03
Flashing Titration #          9
# inversions for batch pblm          29
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
 DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 (=) ATM      Temperature=      2.98E+02 (=) Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.87052148E+01   1.11018564E+02   9.93931709E+01   1.00178579E+05   Hydrogen
  3.67169708E+01   5.55273411E+01   4.97126537E+01   7.95375832E+05   Oxygen
  5.43147475E+00   5.61001696E+00   5.02256990E+00   1.15467727E+05   Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Calcium
  1.95190099E+00   5.59865759E+00   5.01240002E+00   1.77704618E+05   Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Sulfur
  3.47776855E+00   6.18147537E-03   5.53418864E-03   6.64711398E+01   Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   U(VI)
  3.47561578E+00   6.66349238E-06   5.96573175E-06   1.41416597E+00   Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00   Electron
 -1.97029011E-15  -5.65140329E-15  -5.05962251E-15   0.00000000E+00   Charge

  Solution Parameters, Calculated
    SOLUTION MASS      462.933810446941      grams
    H2O MASS           348.637323019306      grams
    TDS(g/kg)          327.837784084038      g/kgH2O

  Specified Solution Density
    DENSITY            1188.79464008680      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.389414449591680       liters
    TDS                293.508593601194      g/l

  Density based on TDS and NaCl solutions     1188.79464008680      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                          Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                          WATER    8.31919E-01   7.78249E-01   0.9355        1.93524E+01   4.96961E+01   8.95286E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s) 9.96914E+00   1.00000E+00    1.000        3.47561E+00   8.92523E+00   3.14209E+06
Na+                           Na+     5.61002E+00   5.28690E+00   0.9424        1.95586E+00   5.02257E+00   1.15468E+05
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
Cl-                              Cl-       5.59866E+00   5.27483E+00   0.9422    1.95190E+00   5.01240E+00   1.77705E+05
CO3=                             CO3=      5.06627E-03   1.31507E-04   2.5957E-02  1.76629E-03   4.53576E-03   2.72187E+02
HCO3-                            HCO3-     1.09867E-03   4.06389E-04   0.3699    3.83037E-04   9.83623E-04   6.00178E+01
OH-                              OH-       1.01865E-04   5.54263E-05   0.5441    3.55141E-05   9.11987E-05   1.55104E+00   -1.56E-10
Np02(CO3)3=4-                    Np02(CO3)3=4-  3.29354E-06  2.65024E-15  8.0468E-10  1.14825E-06  2.94866E-06  1.32417E+00   1.74E-09
Np02(CO3)2=2-                    Np02(CO3)2=2-  3.23222E-06  6.41283E-11  2.6028E-05  1.12687E-06  2.89376E-06  1.12586E+00   8.08E-10
Np02CO3-                         Np02CO3-  1.33806E-07   2.43236E-07   1.818     4.66498E-08   1.19795E-07   3.94192E-02   5.49E-13
CO2(aq)                          CO2(aq)   5.53405E-08   1.60697E-07   2.904     1.92938E-08   4.95456E-08   2.18049E-03   -9.19E-09
Np02+                            Np02+     3.76124E-09   7.45944E-09   1.982     1.31200E-09   3.36917E-09   9.06466E-04   -7.94E-10
Np02OH(aq)                       Np02OH(aq)  1.59617E-10  1.59617E-10  1.000     5.56486E-11   1.42903E-10   4.08781E-05   4.13E-09
H+                               H+        3.62550E-11   1.41496E-10   3.903     1.26398E-11   3.24586E-11   3.27150E-08   -4.92E-09
Np02(OH)2-                       Np02(OH)2-  1.42919E-12  4.26699E-13  0.2986    4.98268E-13   1.27953E-12   1.87777E-07   9.06E-09
HCl(aq).....to.titrate.acid.only  0.00000E+00  0.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
NaOH(aq).....to.titrate.base.only  0.00000E+00  0.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
Np02OH(aged)                     Np02OH(aged)  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
Np02OH(amor)                     Np02OH(amor)  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.68E+00
Na3Np02(CO3)2(s)_DISABLED_DISABLED  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+02
NaCl                             Halite    0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -1.36E-01
NaHCO3                           Nahcolite  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.25E+00
Na2CO3.10H2O                     Natron    0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+00
Na2CO3.7H2O    Na2CO3-Heptahydrate  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.56E+00
Na2CO3.H2O                       Thermonatrite  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.85E+00
Na3H(CO3)2.2H2O                  Trona     0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -4.28E+00

pH (-log[aH+]); pmH(-log[mH+])      9.8493      10.4406
Osmotic Coefficient=     1.240893
Equilibrium RH (%) =    77.824850
Ionic Strength (m) =     5.615126
Density, kg/m3     =     1188.79
fCO2(g); log[fCO2(g)]=                                    4.873E-06    -5.31

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -4.640728732E+03
Flushing Titration #       10
 4 inversions for batch pbln       28 .
Benchmark TITRATE Problem, LOG10 option; Np(V)02 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  NEW84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NEA94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4  (FRE889,FRF890,P91,RFF892,RFF894,RAF894)
     Pressure=      1.00000E+00 (=) ATM     Temperature=      2.98E+02 (=) Kelvin

Elemental Abundances for Flush Problem

  Total Moles      Aq. Molality      Aq. Molarity      Aq. mg/liter

  3.87560135E+01   1.11018653E+02    9.93942650E+01    1.00179480E+05  Hydrogen
  3.67651156E+01   5.55352555E+01    4.97203463E+01    7.95495709E+05  Oxygen
  5.43404174E+00   5.61002728E+00    5.02262026E+00    1.15468885E+05  Sodium
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
  1.95263769E+00   5.59343408E+00    5.00776448E+00    1.77540274E+05  Chlorine
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
  3.47868370E+00   8.80060113E-03    7.87911990E-03    9.46361091E+01  Carbon
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Poslon
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Neglon
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
  1.47561578E+00   1.21872216E-05    1.10901974E-05    2.62891134E+00  Np(V)
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
 -1.61099060E-15  -4.61476789E-15   -4.13157112E-15    0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      463.532138924444      grams
    H2O MASS           349.096609954678      grams
    TDS(g/kg)          327.812362913951      g/kgH2O

  Specified Solution Density
    DENSITY            1188.78161259327      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.389922029424118        liters
    TDS             293.488236965686         g/l

  Density based on TDS and NaCl solutions     1188.78161259327      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                     Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                              WATER     8.31951E-01   7.78350E-01   0.9356    1.93770E+01   4.96966E+01   8.95293E+05
NaNp02CO3(s)                     NaNp02CO3(s)  9.95607E+00  1.00000E+00  1.000     3.47561E+00   8.91361E+00   3.13800E+06
Na+                              Na+       5.61003E+00   5.28539E+00   0.9421    1.95843E+00   5.02262E+00   1.15469E+05
Cl-                              Cl-       5.59343E+00   5.26704E+00   0.9416    1.95264E+00   5.00776E+00   1.77540E+05
CO3=                             CO3=      7.62562E-03   1.97880E-04   2.5949E-02  2.66206E-03   6.82717E-03   4.09693E+02
HCO3-                            HCO3-     1.14291E-03   4.22533E-04   0.3697    3.98983E-04   1.02324E-03   6.24350E+01
OH-                              OH-       1.47379E-04   8.02242E-05   0.5443    5.14493E-05   1.31948E-04   2.24408E+00   -2.20E-08
Np02(CO3)3=4-                    Np02(CO3)3=4-  7.39875E-06  6.00222E-15  8.1125E-10  2.58286E-06  6.62405E-06  2.97469E+00   3.53E-08
Np02(CO3)2=2-                    Np02(CO3)2=2-  4.85191E-06  1.26624E-10  2.6098E-05  1.69378E-06  4.34388E-06  1.69005E+00   1.76E-08
Np02CO3-                         Np02CO3-  1.33905E-07   2.43306E-07   1.817     4.67454E-08   1.19884E-07   3.94486E-02   2.93E-11
CO2(aq)                          CO2(aq)   3.97510E-08   1.15435E-07   2.904     1.38769E-08   3.55888E-08   1.56626E-03   -3.78E-07
Np02+                            Np02+     2.50641E-09   4.95882E-09   1.978     8.74975E-10   2.24398E-09   6.03735E-04   -1.77E-08
Np02OH(aq)                       Np02OH(aq)  1.53583E-10  1.53583E-10  1.000     5.36149E-11   1.37502E-10   3.93329E-05   1.09E-07
H+                               H+        2.51081E-11   9.77709E-11   3.894     8.76512E-12   2.24792E-11   2.26567E-08   -1.27E-07
Np02(OH)2-                       Np02(OH)2-  1.99131E-12  5.94256E-13  0.2984    6.95155E-13   1.78281E-12   5.40300E-07   2.36E-07
HCl(aq).....to.titrate.acid.only  0.00000E+00  0.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
NaOH(aq).....to.titrate.base.only  0.00000E+00  0.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
Np02OH(aged)                     Np02OH(aged)  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.09E+00
Np02OH(amor)                     Np02OH(amor)  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.68E+00
Na3Np02(CO3)2(s)_DISABLED_DISABLED  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+02
NaCl                             Halite    0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -1.36E-01
NaHCO3                           Nahcolite  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.25E+00
Na2CO3.10H2O                     Natron    0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+00
Na2CO3.7H2O    Na2CO3-Heptahydrate  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.56E+00
Na2CO3.H2O                       Thermonatrite  0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.85E+00
Na3H(CO3)2.2H2O                  Trona     0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -4.28E+00

pH (-log[aH+]); pmH(-log[mH+])     10.0098      10.6003
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
Osmotic Coefficient=    1.240532
Equilibrium RH (%) =   77.834968
Ionic Strength (m) =    5.617741
Density, kg/ml     =    1188.78
fCO2(g); log[fCO2(g)]=                                    3.501E-06    -5.46

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergance criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.64367246E+03
Flashing Titration #          11
# inversions for batch pblm          28
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFT94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.88284068E+01   1.11018771E+02   9.93954956E+01   1.00180724E+05  Hydrogen
  3.68052248E+01   5.55465070E+01   4.97209848E+01   7.95665918E+05  Oxygen
  5.43746997E+00   5.61004415E+00   5.02269243E+00   1.15470544E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95368755E+00   5.58601315E+00   5.00117739E+00   1.77306742E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  1.47998788E+00   1.25239828E-02   1.12127662E-02   1.34676535E+02  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  1.47561578E+00   2.32128943E-05   2.07825866E-05   4.92647475E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.72202137E-15  -4.92362968E-15  -4.40814312E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     464.385150217376      grams
    H2O MASS          349.746321818895      grams
    TDS(g/kg)         327.777080834728      g/kgH2O

  Specified Solution Density
    DENSITY           1188.76353136245      kg/m^3 * g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.390645521977900       liters
    TDS               293.459983409118      g/l

  Density based on TDS and NaCl solutions    1188.76353136245      g/l
  Percent relative error vs NaCl density     0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                  WATER  8.31997E-01   7.78493E-01   0.9357        1.94140E+01   4.96971E+01   8.95304E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.93751E+00   1.00000E+00    1.000        3.47561E+00   8.89709E+00   3.13218E+06
Na+                                  Na+    5.61004E+00   5.28333E+00   0.9418        1.96209E+00   5.02269E+00   1.15471E+05
Cl-                                  Cl-    5.58601E+00   5.25591E+00   0.9409        1.95369E+00   5.00118E+00   1.77307E+05
CO3=                                 CO3=   1.12609E-02   2.92079E-04   2.5937E-02    3.93846E-03   1.00819E-02   6.05009E+02
HCO3-                                HCO3-  1.20082E-03   4.43607E-04   0.3694        4.19981E-04   1.07510E-03   6.55992E+01
OH-                                  OH-    2.07123E-04   1.12810E-04   0.5447        7.24404E-05   1.85438E-04   3.15380E+00   -2.21E-09
NpO2(CO3)3---        NpO2(CO3)3---   1.59398E-05   1.30821E-14   8.2072E-10    5.57490E-06   1.42710E-05   6.40874E+00   8.63E-09
NpO2(CO3)2=-          NpO2(CO3)2=-   7.13717E-06   1.86975E-10   2.6197E-05    2.49620E-06   6.38993E-06   2.48610E+00   4.17E-09
NpO2CO3-                  NpO2CO3-   1.34044E-07   2.43401E-07   1.816         4.68815E-08   1.20010E-07   3.94902E-02   8.13E-12
CO2(aq)                    CO2(aq)   2.96765E-08   8.61856E-08   2.904         1.03792E-08   2.65695E-08   1.16932E-03   -9.13E-08
NpO2+                        NpO2+   1.70329E-09   3.36086E-09   1.973         5.95718E-10   1.52496E-09   4.10285E-04   -6.21E-09
NpO2OH(aq)                NpO2OH(aq)   1.46370E-10   1.46370E-10   1.000         5.11925E-11   1.31046E-10   3.74863E-05   4.07E-08
H+                                   H+     1.79163E-11   6.95424E-11   3.882         6.26615E-12   1.60405E-11   1.61672E-08   -4.49E-08
NpO2(OH)2-                NpO2(OH)2-   2.67040E-12   7.96388E-13   0.2982        9.33963E-13   2.39082E-12   7.24565E-07   8.56E-08
HCl(aq).....to.titrate.acid.only     0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02
NaOH(aq).....to.titrate.base.only    0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
NpO2OH(aged)_____________NpO2OH(aged)   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.11E+00
NpO2OH(amor)_____________NpO2OH(amor)   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.70E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+02
NaCl_____________________________Halite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.27E-01
NaHCO3___________________________Nahcolite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.23E+00
Na2CO3.10H2O_____________________Natron   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.35E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.39E+00
Na2CO3.H2O_____________Thermonatrite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.68E+00
Na3H(CO3)2.2H2O_________________Trona   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.89E+00

pH (-log[aH+]); pmH(-log[mH+])     10.1578       10.7468
Osmotic Coefficient=    1.240021
Equilibrium RH (%) =   77.849336
Ionic Strength (m) =    5.621486
Density, kg/m3     =    1188.76
fCO2(g); log[fCO2(g)]=                                    2.614E-06    -5.58

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.64786705E+03
Flashing Titration #          12
# inversions for batch pblm          28
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFT94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
 3.89315747E+01   1.11018623E+02   9.93971848E+01   1.00182423E+05  Hydrogen
 3.68623846E+01   5.55624877E+01   4.97460679E+01   7.95907238E+05  Oxygen
 5.44291331E+00   5.61007256E+00   5.02279611E+00   1.15472927E+05  Sodium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
 1.95518372E+00   5.57548446E+00   4.99182884E+00   1.76975308E+05  Chlorine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
 3.48184647E+00   1.78114648E-02   1.59469162E-02   1.91538411E-02  Carbon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
 3.47561578E+00   4.37690919E-05   3.91872342E-05   9.28926332E+00  Np(V)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
-1.77023110E-15  -5.04806576E-15  -4.51962164E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS      465.601420606259      grams
   H2O MASS           350.675126352089      grams
   TDS(g/kg)          327.728674256698      g/kgH2O

 Specified Solution Density
   DENSITY            1188.73872346794      kg/m^3 * g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL    0.391676034795075        liters
   TDS             293.421218832867         g/l

 Density based on TDS and NaCl solutions    1188.73872346794      g/l
 Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                          Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                          WATER    8.32061E-01   7.78697E-01   0.9359        1.94655E+01   4.96979E+01   8.95318E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)         9.91117E+00   1.00000E+00   1.000         3.47560E+00   8.87364E+00   3.12393E+06
Na+                          Na+      5.61007E+00   5.28057E+00   0.9413        1.96731E+00   5.02280E+00   1.15473E+05
Cl-                          Cl-      5.57548E+00   5.24002E+00   0.9398        1.95518E+00   4.99183E+00   1.76975E+05
CO3=                         CO3=     1.64154E-02   4.25480E-04   2.5920E-02    5.75648E-03   1.46970E-02   8.81956E+02
HCO3-                        HCO3-    1.27533E-03   4.70618E-04   0.3690        4.47227E-04   1.14183E-03   6.96709E+01
OH-                          OH-      2.84255E-04   1.54942E-04   0.5451        9.96812E-05   2.54499E-04   4.32833E+00   -1.39E-09
NpO2(CO3)3==-          NpO2(CO3)3==-  3.32873E-05   2.77756E-14   8.3442E-10    1.16730E-05   2.98027E-05   1.33636E+01    5.09E-09
NpO2(CO3)2=-           NpO2(CO3)2=-   1.03463E-05   2.72515E-10   2.6339E-05    3.62818E-06   9.26320E-06   3.60399E+00    2.40E-09
NpO2CO3-                 NpO2CO3-     1.34242E-07   2.43528E-07   1.814         4.70755E-08   1.20190E-07   9.95491E-02    6.17E-12
CO2(aq)                    CO2(aq)    2.29199E-08   6.65707E-08   2.904         8.03744E-09   2.05206E-08   9.01107E-04   -7.33E-08
NpO2+                        NpO2+    1.17432E-09   2.30833E-09   1.966         4.11805E-10   1.05139E-09   2.82874E-04   -2.44E-09
NpO2OH(aq)              NpO2OH(aq)    1.38078E-10   1.38078E-10   1.000         4.84205E-11   1.23624E-10   3.53631E-05    3.36E-08
H+                              H+    1.31074E-11   5.06455E-11   3.864         4.59643E-12   1.17353E-11   1.18280E-08   -1.61E-08
NpO2(OH)2-             NpO2(OH)2-    3.46327E-12   1.03185E-12   0.2979        1.21448E-12   3.10073E-12   9.39711E-07    6.97E-08
HCl(aq).....to.titrate.acid.only     0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02
NaOH(aq).....to.titrate.base.only    0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
NpO2OH(aged)_____NpO2OH(aged)        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.13E+00
NpO2OH(amor)_____NpO2OH(amor)        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.73E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+02
NaCl_____________________Halite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.28E-01
NaHCO3___________________Nahcolite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.20E+00
Na2CO3.10H2O_____________Natron      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.19E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.23E+00
Na2CO3.H2O_____Thermonatrite         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+00
Na3H(CO3)2.2H2O__________Trona       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.70E+00

pH (-log[aH+]); pmH(-log[mH+])     10.2955      10.8825
Osmotic Coefficient=    1.239297
Equilibrium RH (%) =   77.869707
Ionic Strength (m) =    5.626852
Density, kg/m3     =    1188.74
fCO2(g); log[fCO2(g)]=                                  2.019E-06    -5.69

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -4.65384406E+03
Flushing Titration #          13
# inversions for batch pblm          28
1Benchmark TITRATE Problem, LOG10 option; Np(V)02 with CO3 in 5.61molal NaCl   FMT V2.3
 DATABASE:  HDNB6/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RPF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flush Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

 3.90785996E+01   1.11019115E+02   9.93994493E+01   1.00184705E+05  Hydrogen
 3.69438430E+01   5.55851538E+01   4.97674088E+01   7.96248680E+05  Oxygen
 5.45034267E+00   5.61012129E+00   5.02294553E+00   1.15476363E+05  Sodium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
 1.95731591E+00   5.56057489E+00   4.97858483E+00   1.76505768E+05  Chlorine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
 3.48649515E+00   2.53082323E-02   2.26593804E-02   2.72161818E+02  Carbon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
 3.47561578E+00   8.26620364E-05   7.40103261E-05   1.75440146E+01  Np(V)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
-1.64947808E-15  -4.68603272E-15  -4.19557544E-15   0.00000000E+00  Charge
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  Solution Parameters, Calculated
    SOLUTION MASS      467.335943430018       grams
    H2O MASS           351.998839687452       grams
    TDS(g/kg)          327.663306631852       g/kgH2O

  Specified Solution Density
    DENSITY            1188.70522197651       kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.393147043346002        liters
    TDS                291.368869726077       g/l

  Density based on TDS and NaCl solutions     1188.70522197651       g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                WATER      8.32153E-01   7.78985E-01   0.9361        1.95390E+01   4.96989E+01   8.95336E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)        9.67186E+00   1.00000E+00   1.000         3.47559E+00   8.84042E+00   3.11224E+06
Na+                                Na+        5.61012E+00   5.27693E+00   0.9406        1.97476E+00   5.02295E+00   1.15476E+05
Cl-                                Cl-        5.56057E+00   5.21732E+00   0.9383        1.95732E+00   4.97858E+00   1.76506E+05
CO3=                               CO3=       2.37058E-02   6.13801E-04   2.5892E-02    8.34440E-03   2.12246E-02   1.27367E+03
HCO3-                              HCO3-      1.36956E-03   5.04583E-04   0.3684        4.82083E-04   1.22622E-03   7.48201E+01
OH-                                OH-        3.82200E-04   2.08552E-04   0.5457        1.34534E-04   3.42198E-04   5.81986E+00   -1.15E-09
NpO2(CO3)3=5-          NpO2(CO3)3=5-      6.77047E-05   5.78442E-14   8.5436E-10    2.38320E-05   6.06184E-05   2.72222E+01    3.43E-09
NpO2(CO3)2-2-          NpO2(CO3)2-2-      1.48219E-05   3.93404E-10   2.6542E-05    5.21729E-06   1.32706E-05   5.16313E+00    1.57E-09
NpO2CO3-                   NpO2CO3-       1.34522E-07   2.43696E-07   1.812         4.73516E-08   1.20442E-07   3.96323E-02    5.30E-12
CO2(aq)                        CO2(aq)    1.82542E-08   5.30275E-08   2.905         6.42544E-09   1.63436E-08   7.19279E-04   +6.76E-08
NpO2+                              NpO2+      8.18986E-10   1.60121E-09   1.955         2.88282E-10   7.33267E-10   1.97283E-04   +1.63E-09
NpO2OH(aq)                 NpO2OH(aq)     1.28920E-10   1.28920E-10   1.000         4.53797E-11   1.15427E-10   3.30103E-05    3.13E-08
H+                                 H+         9.80463E-12   3.76405E-11   3.839         3.45122E-12   8.77844E-12   8.86779E-09   -3.29E-08
NpO2(OH)2-                 NpO2(OH)2-     4.35852E-12   1.29676E-12   0.2975        1.53419E-12   3.90234E-12   1.18265E-06    6.42E-08
HCl(aq).....to.titrate.acid.only           0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   +2.50E+02
NaOH(aq).....to.titrate.base.only          0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
NpO2OH(aged)_____________NpO2OH(aged)      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.16E+00
NpO2OH(amor)_____________NpO2OH(amor)      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.76E+00
NaINpO2(CO3)2(s)_DISABLED_DISABLED         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+02
NaCl_____________________Halite            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.31E-01
NaHCO3___________________Nahcolite         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.17E+00
Na2CO3.10H2O_____________Natron            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.03E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.07E+00
Na2CO3.H2O_____________Thermonatrite       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.36E+00
Na3H(CO3)2.2H2O_____________Trona          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.51E+00

pH (-log(aH+)); pmH(-log[mH+])      10.4243       11.0086
Osmotic Coefficient=     1.238276
Equilibrium RH (%) =    77.898521
Ionic Strength (m) =     5.634549
Density, kg/m3     =     1188.71
fCO2(g); log(fCO2(g))=                                  1.608E-06    -5.79

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -4.66236092E+03
Flashing Titration #          14
# inversions for batch pblm          28
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.6lmolal NaCl   FMT V2.3
DATABASE:  HDNB6/FWS6; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,PRF90,P91,RPFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

  Elemental Abundances for Flash Problem

    Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

    3.92881252E+01    1.11019354E+02    9.94024309E+01    1.00187710E+05  Hydrogen
    3.70599297E+01    5.56172351E+01    4.97975186E+01    7.96730419E+05  Oxygen
    5.46093075E+00    5.61020635E+00    5.02316152E+00    1.15481328E+05  Sodium
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
    1.96035450E+00    5.53953836E+00    4.95987023E+00    1.75842779E+05  Chlorine
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
    3.48826979E+00    3.59127333E-02    3.21548707E-02    3.86212152E+02  Carbon
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  PosIon
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  NegIon
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Th(IV)
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
    3.47561578E+00    1.55346593E-04    1.39091324E-04    3.29713479E+01  Np(V)
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
   -1.58811224E-15   -4.48764594E-15   -4.01806440E-15    0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      469.810029265022       grams
    H2O MASS           353.885368468190       grams
    TDS(g/kg)          327.576868460591       g/kgH2O

  Specified Solution Density
    DENSITY            1188.66091947607       kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.395243102189397        liters
    TDS                291.299643066970       g/l

  Density based on TDS and NaCl solutions     1188.66091947607       g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                WATER      8.32282E-01   7.79391E-01   0.9365        1.96437E+01   4.97003E+01   8.95361E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)        9.82115E+00   1.00000E+00   1.000         3.47556E+00   8.79348E+00   3.09571E+06
Na+                                Na+        5.61021E+00   5.27230E+00   0.9398        1.98537E+00   5.02316E+00   1.15481E+05
Cl-                                Cl-        5.53952E+00   5.18493E+00   0.9360        1.96035E+00   4.95987E+00   1.75842E+05
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
CO3=                          CO3=      3.39812E-02  8.78458E-04  2.5851E-02  1.20255E-02  3.04255E-02  1.82581E+03
HCO3-                         HCO3-     1.48672E-03  5.46468E-04  0.3676      5.26128E-04  1.33115E-03  8.12230E+01
OH-                           OH-       5.04619E-04  2.75741E-04  0.5464      1.78577E-04  4.51816E-04  7.68417E+00   -1.19E-09
NpO2(CO3)3=5-          NpO2(CO3)3=5-     1.34208E-04  1.18584E-13  8.8359E-10  4.74943E-05  1.20165E-04  5.39629E+01    2.60E-09
NpO2(CO3)2=4-          NpO2(CO3)2=4-     2.10028E-05  5.63525E-10  2.6831E-05  7.43260E-06  1.88051E-05  7.31643E+00    1.17E-09
NpO2CO3-                    NpO2CO3-    1.34916E-07  2.43910E-07  1.808       4.77447E-08  1.20798E-07  3.97494E-02    5.27E-12
CO2(aq)                       CO2(aq)   1.49488E-08  4.34356E-08  2.906       5.29018E-09  1.33846E-08  5.89054E-04   -7.10E-08
NpO2+                         NpO2+     5.77122E-10  1.11979E-09  1.940       2.04235E-10  5.16733E-10  1.39025E-04   -1.24E-09
NpO2OH(aq)               NpO2OH(aq)     1.19205E-10  1.19205E-10  1.000       4.21850E-11  1.06732E-10  3.05311E-05    3.24E-08
H+                            H+        7.48733E-12  2.84836E-11  3.804       2.64966E-12  6.70384E-12  6.75682E-09   -3.36E-08
NpO2(OH)2-               NpO2(OH)2-     5.33952E-12  1.58534E-12  0.2969      1.88958E-12  4.78080E-12  1.44884E-06    6.60E-08
HCl(aq).....to.titrate.acid.only        0.00000E+00  0.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -2.50E+02
NaOH(aq).....to.titrate.base.only       0.00000E+00  0.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -2.50E+02
NpO2OH(aged)_____________NpO2OH(aged)   0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -2.93E+02
NpO2OH(amor)_____________NpO2OH(amor)   0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -3.20E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED      0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -3.79E+00
NaCl_____________________Halite         0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   +9.30E+02
NaHCO3___________________Nahcolite      0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -1.34E-01
Na2CO3.10H2O_____________Natron         0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -2.14E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate      0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -1.67E+00
Na2CO3.H2O_______Thermonatrite          0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -1.91E+00
Na3H(CO3)2.2H2O_____________Trona       0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00   -2.20E+00
                                                                                                                      -3.32E+00

pH (-log[aH+]); pmH(-log[mH+])     10.5454      11.1257
Osmotic Coefficient=     1.236838
Equilibrium RH (%) =    77.939147
Ionic Strength (m) =     5.645593
Density, kg/m3     =    1188.66
fCO2(g); log[fCO2(g)]=                                    1.317E-06    -5.88

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -6.67449693E+03
Flushing Titration #          15
# inversions for batch pbim          28
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl    FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (HR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flush Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

  3.95867206E+01    1.11019649E+02    9.94062599E+01    1.00191569E+05  Hydrogen
  3.72253652E+01    5.56624986E+01    4.98398335E+01    7.97407433E+05  Oxygen
  5.47601956E+00    5.61035435E+00    5.02347422E+00    1.15488517E+05  Sodium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
  1.96468480E+00    5.50989354E+00    4.93352227E+00    1.74908165E+05  Chlorine
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
  3.49364905E+00    5.08618173E-02    4.55413352E-02    5.46986977E+02  Carbon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  PosIon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  NegIon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Th(IV)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
  3.47561578E+00    2.88102498E-04    2.57965074E-04    6.11501564E+01  Np(V)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
 -1.36636579E-15   -3.83192766E-15   -3.43108273E-15    0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     473.339684533624      grams
    H2O MASS          356.574003417585      grams
    TDS(g/kg)         327.465491025420      g/kgH2O

  Specified Solution Density
    DENSITY           1188.60383111845      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.398231666549673       liters
    TDS               293.210437350980      g/l

  Density based on TDS and NaCl solutions    1188.60383111845      g/l
  Percent relative error vs NaCl density    0.00000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                          Molality      Activity      Act Coef      Total Moles    Molarity      mg/liter      Descriptor

H2O                          WATER    8.32465E-01   7.79962E-01   0.9369        1.97930E+01   4.97021E+01   8.95393E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)  9.74696E+00   1.00000E+00   1.000         3.47551E+00   8.72736E+00   3.07243E+06
Na+                           Na+       5.61035E+00   5.26665E+00   0.9387        2.00051E+00   5.02347E+00   1.15489E+05
Cl-                           Cl-       5.50985E+00   5.13884E+00   0.9327        1.96468E+00   4.93352E+00   1.74908E+05
CO3=                          CO3=      4.83871E-02   1.24807E-03   2.5788E-02    1.72571E-02   4.33344E-02   2.60046E+03
HCO3-                         HCO3-     1.63010E-03   5.97114E-04   0.3663        5.81251E-04   1.45958E-03   8.90593E+01
OH-                           OH-       6.55397E-04   3.58792E-04   0.5474        2.33698E-04   5.86839E-04   9.98054E+00   -1.51E-09
NpO2(CO3)3=5-          NpO2(CO3)3=5-     2.58546E-04   2.39623E-13   9.2681E-10    9.21906E-05   2.31500E-04   1.03961E+02    2.16E-09
NpO2(CO3)2=4-          NpO2(CO3)2=4-     2.94209E-05   8.01487E-10   2.7242E-05    1.04907E-05   2.63433E-05   1.02493E+01    9.59E-10
NpO2CO3-                    NpO2CO3-    1.35468E-07   2.44172E-07   1.802         4.83043E-08   1.21297E-07   3.99135E-02    6.05E-12
CO2(aq)                       CO2(aq)   3.64751E-08   8.87045E-08   2.907         4.47472E-09   1.12365E-08   4.94515E-04   -8.59E-08
NpO2+                         NpO2+     4.11022E-10   7.89015E-10   1.920         1.46560E-10   3.68027E-10   9.90165E-05   -1.06E-09
NpO2OH(aq)               NpO2OH(aq)     1.09291E-10   1.09291E-10   1.000         3.89705E-11   9.78589E-11   2.79929E-05    3.66E-08
NpO2(OH)2-               NpO2(OH)2-     6.38945E-12   1.89128E-12   0.2960        2.27831E-12   5.72107E-12   1.73384E-06    7.43E-08
H+                            H+        5.63272E-12   2.19064E-11   3.756         2.07980E-12   5.22258E-12   5.26384E-09   -3.76E-08
HCl(aq).....to.titrate.acid.only        0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02
NaOH(aq).....to.titrate.base.only       0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.93E+02
NpO2OH(aged)_____________NpO2OH(aged)   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.23E+00
NpO2OH(amor)_____________NpO2OH(amor)   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.83E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+02
NaCl_____________________Halite         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.38E-01
NaHCO3___________________Nahcolite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.16E+00
Na2CO3.10H2O_____________Natron         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.72E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.76E+00
Na2CO3.H2O_______Thermonatrite          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.05E+00
Na3H(CO3)2.2H2O_____________Trona       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.13E+00

pH (-log[aH+]); pmH(-log[mH+])     10.6594      11.2341
Osmotic Coefficient=     1.234823
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
1975  Equilibrium RH (%) =   77.996177
1976  Ionic Strength (m) =    5.661425
1977  Density, kg/m3     =    1188.60
1978  fCO2(g); log(fCO2(g))=                                  1.106E-06    -5.96
1979
1980  NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
1981          - Gas "molality" and "activity" are gas partial pressures
1982          - "Descriptor" means:
1983            "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
1984            "Saturation Index for minerals, SI=log10(IAP/Ksp)
1985            "log10(activity) for aqueous species with very small concentrations
1986            "log10(partial pressure) for gases
1987
1988  Total G/RT=    -4.69179003E+03
1989  TITRATE  file name is U1:[SCBARB.FMT.UM]NP_NACL_BM_LOG.TITRATE;1
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

See Table 15 for explanation of this listing.

```
INPUT    file name is:U1:[SCBABB.FMT.UM]NP_NACL_BM_LIN.IN;1
INGUESS  file name is:U1:[SCBABB.FMT.UM]NP_NACL_BM_LIN.INGUESS;1
OUTPUT   file name is:U1:[SCBABB.FMT.UM]NP_NACL_BM_LIN.OUT;1
CHEMDAT  file name is U1:[SCBABB.FMT.UM]FMT_JOM_NP_AM_RTEST.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

Accuracy of reactions is              1.0000E-06
Minimum elemental abundance is        1.0000E-18
Number of Aqueous Species is          50

PITZER Data Base NOT Echoed in this Run

Species Order for Pitzer Parameters

Cations    13

Na+              K+               Ca++             Mg++             MgOH+            H+
MgB(OH)4+        CaB(OH)4+        Am+++            AmCO3+           Th++++           UO2++
NpO2+

Anions     20

Cl-              SO4=             HSO4-            OH-              HCO3-            CO3=
B(OH)4-          BJO3(OH)4-       B4O5(OH)4=       Br-              Am(CO3)2-        Am(CO3)3=-
ClO4-         pe NpO2(OH)2-       NpO2CO3-         NpO2(CO3)2=-     NpO2(CO3)3=-=    H2PO4-
HPO4=            PO4=-

Neutral    6

CO2(aq)          CaCO3(aq)        MgCO3(aq)        B(OH)3(aq)       NpO2OH(aq)       H3PO4(aq)

using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

this is a TITRATION problem

Ideal Gas Constant is Unity (Dimensionless)
Temperature =      298.15 [=] degree Kelvin

  115 Species                    23 Elements

          Element Name      Molecular Weight
          Hydrogen             1.00790
          Oxygen              15.99940
          Sodium              22.98977
          Potassium           39.09830
          Magnesium           24.30500
          Calcium             40.08000
          Chlorine            35.45300
          Sulfur              32.06000
          Carbon              12.01100
          PosIon               0.00000
          NegIon               0.00000
          Air                 28.84000
          Boron               10.81000
          Bromine             79.90400
          TracerEl             0.00000
          Th(IV)             232.03810
          Am(III)            243.00000
          U(VI)              238.02900
          Np(V)              237.04820
          ClO4-(EL)           99.45060
          Phosphorus          30.97400
          Electron             0.00000
          Charge               0.00000

    Species Name                          Phase      Mol.Wt.   Std Chemical Potential, u/RT
  1 H2O                          WATER    aqueous     18.015      -95.6635
  2 Na+                          Na+      aqueous     22.990     -105.6510
  3 K+                           K+       aqueous     39.098     -113.9570
  4 Ca++                         Ca++     aqueous     40.080     -223.3000
  5 Mg++                         Mg++     aqueous     24.305     -183.4680
  6 MgOH+                        MgOH+    aqueous     41.312     -251.9400
  7 H+                           H+       aqueous      1.008        0.0000
  8 Cl-                          Cl-      aqueous     35.453      -52.9550
  9 SO4=                         SO4=     aqueous     96.058     -300.3860
 10 HSO4-                        HSO4-    aqueous     97.066     -304.9420
 11 OH-                          OH-      aqueous     17.007      -63.4350
 12 HCO3-                        HCO3-    aqueous     61.017     -236.7510
 13 CO3=                         CO3=     aqueous     60.009     -212.9440
 14 CO2(aq)                      CO2(aq)  aqueous     44.010     -155.6800
 15 CaCO3(aq)                    CaCO3(aq) aqueous    100.089     -443.5000
 16 MgCO3(aq)                    MgCO3(aq) aqueous    84.314      -403.1550
 17 B(OH)3(aq)                   B(OH)3(aq) aqueous   61.832      -390.8100
 18 B(OH)4-                      B(OH)4-  aqueous     78.839      -465.2000
 19 BJO3(OH)4-                   BJO3(OH)4- aqueous   148.457     -963.7700
 20 B4O5(OH)4=                   B4O5(OH)4= aqueous   191.266    -1239.1000
 21 CaB(OH)4+                    CaB(OH)4+ aqueous    118.919     -692.3000
 22 MgB(OH)4+                    MgB(OH)4+ aqueous    103.144     -651.8900
 23 Br-                          Br-      aqueous     79.904      -999.9900
 24 ClO4-            perchlorate ClO4-    aqueous     99.451      -999.9900
 25 NaOH(aq).....to.titrate.base.only     aqueous     39.997       500.0000
 26 HCl(aq).....to.titrate.acid.only      aqueous     36.461       500.0000
 27 HClO4(aq)....to.titrate.acid.only     aqueous    100.459       500.0000
 28 PosIon.............POSITIVE.ION       aqueous      0.000         0.0000
 29 NegIon.............NEGATIVE.ION       aqueous      0.000         0.0000
 30 PosIon(OH)(aq).....to.titrate.base     aqueous     17.007       500.0000
 31 HNegIon(aq).....to.titrate.acid        aqueous      1.008       500.0000
 32 Tracer(aq).....conservative.tracer     aqueous      0.000         0.0000
 ?? H3PO4(aq)                   H3PO4(aq) aqueous     ??.???      -???.????
 34 H2PO4-                      H2PO4-   aqueous     96.987      -455.9600
 35 HPO4=                       HPO4=    aqueous     95.980      -439.3670
 36 PO4=-                       PO4=-    aqueous     94.972      -410.9470
 37 NpO2+                       NpO2+    aqueous    269.047      -369.1270
 38 NpO2OH(aq)                  NpO2OH(aq) aqueous   286.054     -438.5180
 39 NpO2(OH)2-                  NpO2(OH)2- aqueous   303.062     -505.8290
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

115	40	NpO2CO3-	NpO2CO3-	aqueous	329.056	-594.4920	
116	41	NpO2(CO3)2e-	NpO2(CO3)2e-	aqueous	389.065	-808.4020	
117	42	NpO2(CO3)3eee-	NpO2(CO3)3eee-	aqueous	449.075	-1019.9180	
118	43	Am+++	Am+++	aqueous	243.000	-241.6940	
119	44	AmCO3+	AmCO3+	aqueous	303.009	-472.0600	
120	45	Am(CO3)2-	Am(CO3)2-	aqueous	363.018	-695.8800	
121	46	Am(CO3)3e-	Am(CO3)3e-	aqueous	423.028	-915.4600	
122	47	Am(OH)2+	Am(OH)2+	aqueous	277.015	-393.6470	
123	48	Am(OH)3(aq)	Am(OH)3(aq)	aqueous	294.022	-462.9500	
124	49	Th++++	Th++++	aqueous	232.038	-999.9900	
125	50	UO2++	U(VI)O2++	aqueous	270.028	-999.9900	
126	51	NpO2OH(aged)	NpO2OH(aged)	solid	286.054	-454.0100	
127	52	NpO2OH(amor)	NpO2OH(amor)	solid	286.054	-452.6420	
128	53	NaNpO2CO3(s)	NaNpO2CO3(s)	solid	352.046	-713.7070	
129	54	Na3NpO2(CO3)2(s)	DISABLED_DISABLED	solid	458.035	999.9900	
130	55	AmOHCO3(c)	AmOHCO3(c)	solid	320.017	-569.9800	
131	56	Am(OH)3(s)	Am(OH)3(s)	solid	294.022	-492.2940	
132	57	NaAm(CO3)2.6H2O(c)		solid	494.099	-1396.4940	
133	58	AmPO4(c)	AmPO4(c)	solid	337.972	-709.7500	
134	59	CaSO4	Anhydrite	solid	136.138	-533.7300	
135	60	NaK3(SO4)2	Aphthitalite/Glaserite	solid	332.400	-1057.0500	
136	61	CaCl2.6H2O	Antarcticite	solid	219.077	-893.6500	
137	62	CaCO3	Aragonite	solid	100.089	-455.1700	
138	63	K2SO4	Arcanite	solid	174.256	-532.3900	
139	64	MgCl2.6H2O	Bischofite	solid	203.302	-853.1000	
140	65	Na2Mg(SO4)2.4H2O	Bloedite	solid	334.461	-1383.6000	
141	66	Mg(OH)2	Brucite	solid	58.320	-335.4000	
142	67	Na6CO3(SO4)2	Burkeite	solid	390.063	-1449.4000	
143	68	CaCO3	Calcite	solid	100.089	-455.6000	
144	69	CaCl2.4H2O	CaCl2_Tetrahydrite	solid	183.047	-698.7000	
145	70	Ca4Cl2(OH)6.13H2O	CaOxychloride A	solid	567.467	-2658.4500	
146	71	Ca2Cl2(OH)2.H2O	CaOxychloride B	solid	203.096	-778.4100	
147	72	KMgCl3.6H2O	Carnallite	solid	277.854	-1020.3000	
148	73	MgSO4.7H2O	Epsomite	solid	246.469	-1157.8300	
149	74	CaNa2(CO3)2.5H2O	Gaylussite	solid	296.154	-1360.5000	
150	75	Na2Ca(SO4)2	Glaubarite	solid	278.175	-1047.4500	
151	76	CaSO4.2H2O	Gypsum	solid	172.168	-725.5600	
152	77	NaCl	Halite	solid	58.443	-154.9900	
153	78	MgSO4.6H2O	Hexahydrite	solid	228.454	-1061.6000	
154	79	KMgClSO4.3H2O	Kainite	solid	248.960	-938.2000	
155	80	KHCO3	Kalicinite	solid	100.115	-350.0600	
156	81	MgSO4.H2O	Kieserite	solid	138.378	-579.8000	
157	82	K2Mg(SO4)2.4H2O	Leonite	solid	366.678	-1403.9700	
158	83	Na4Ca(SO4)3.2H2O	Labile_Salt	solid	456.242	-1751.4500	
159	84	MgCO3	Magnesite	solid	84.314	-414.4500	
160	85	Mg2Cl(OH)3.4H2O	MgOxychloride	solid	207.146	-1029.6000	
161	86	KHSO4	Mercallite	solid	136.164	-417.5700	
162	87	Na2SO4.10H2O	Mirabilite	solid	322.189	-1471.1500	
163	88	K8H6(SO4)7	Misenite	solid	991.237	-3039.2400	
164	89	NaHCO3	Nahcolite	solid	84.007	-343.3300	
165	90	Na2CO3.10H2O	Natron	solid	286.141	-1382.7800	
166	91	MgCO3.3H2O	Nesquehonite	solid	138.360	-695.3000	
167	92	K2Mg(SO4)2.6H2O	Picromerite/Schoen	solid	402.708	-1596.1000	
168	93	Na2Ca(CO3)2.2H2O	Pirssonite	solid	242.108	-1073.1000	
169	94	K2MgCa2(SO4)4.2H2O	Polyhalite	solid	602.922	-2282.5000	
170	95	Ca(OH)2	Portlandite	solid	74.095	-362.1200	
171	96	K2CO3.3/2H2O	Potassium_Carbonate	solid	165.229	-577.3700	
172	97	K8H4(CO3)6.3H2O	K-Sequicarbonate	solid	730.919	-2555.4000	
173	98	KNaCO3.6H2O	K-Na-Carbonate	solid	230.188	-1006.8000	
174	99	K2NaH(CO3)2.2H2O	Potassium_Trona	solid	258.243	-971.7400	
175	100	K3H(SO4)2	Sesquipotassium_Sulfate	solid	310.418	-950.8000	
176	101	NaJH(SO4)2	Sesquisodium_Sulfate	solid	262.092	-919.6000	
177	102	Na2CO3.7H2O	Na2CO3-Heptahydrate	solid	232.095	-1094.9500	
178	103	KCl	Sylvite	solid	74.551	-164.8400	
179	104	K2Ca(SO4)2.H2O	Syngenite	solid	328.407	-1164.8000	
180	105	Mg2CaCl6.12H2O	Tachyhydrite	solid	517.590	-2015.9000	
181	106	Na2SO4	Thenardite	solid	142.037	-512.3500	
182	107	Na2CO3.H2O	Thermonatrite	solid	124.004	-518.8000	
183	108	NaJH(CO3)2.2H2O	Trona	solid	226.026	-960.3800	
184	109	Na2B4O7.10H2O	Borax	solid	381.367	-2224.1600	
185	110	B(OH)3	Borix_Acid_Solid	solid	61.832	-390.8800	
186	111	KB5O8.4H2O	K-Pentaborate_(30_C)	solid	293.204	-1770.2600	
187	112	K2B4O7.4H2O	K-Tetraborate_(30_C)	solid	305.493	-1663.4700	
188	113	NaBO2.4H2O	Sodium_Metaborate	solid	137.859	-761.4200	
189	114	NaB5O8.5H2O	Sodium_Pentaborate	solid	295.111	-1854.8000	
190	115	NaBO2.NaCl.2H2O	Teepleite_(20_C)	solid	160.272	-725.7700	

		Truncated Name	Formula Matrix																							
194	1	H2O	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
195	2	Na+	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
196	3	K+	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
197	4	Ca++	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
198	5	Mg++	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
199	6	MgOH+	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
200	7	H+	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
201	8	Cl-	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
202	9	SO4=	0	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2
203	10	HSO4-	1	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
204	11	OH-	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
205	12	HCO3-	1	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
206	13	CO3=	0	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2
207	14	CO2(aq)	0	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
208	15	CaCO3(aq)	0	3	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
209	16	MgCO3(aq)	0	3	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
210	17	B(OH)3(aq)	3	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
211	18	B(OH)4-	4	4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
212	19	B3O3(OH)4-	4	7	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	-1
213	20	B4O5(OH)4=	4	9	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	-2
214	21	CaB(OH)4+	4	4	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
215	22	MgB(OH)4+	4	4	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
216	23	Br-	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
217	24	ClO4- pe	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	-1
218	25	NaOH(aq).....to.ti	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
219	26	NCl(aq).....to.ti	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
220	27	NClO4(aq).....to.ti	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
221	28	PosIon.....	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1
222	29	NegIon.....	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	-1
223	30	PosIon(OH)(aq).....	1	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
224	31	HNegIon(aq).....	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
225	32	Tracer(aq).....cons	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
226	33	H3PO4(aq)	3	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
227	34	H2PO4-	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-1
228	35	HPO4=	1	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-2
229	36	PO4=-	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-3
230	37	NpO2+	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1
231	38	NpO2OH(aq)	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
232	39	NpO2(OH)2-	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-1
233	40	NpO2CO3-	0	5	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-1
234	41	NpO2(CO3)2e-	0	8	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-3
235	42	NpO2(CO3)3eee-	0	11	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-5
236	43	Am+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	3
237	44	AmCO3+	0	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
238	45	Am(CO3)2-	0	6	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	-1

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
  46 Am(CO3)3--              0  3  0  0  0  0  0  0  0  3  0  0  0  0  0  0  0  1  0  0  0  0  0 -3
  47 Am(OH)2+                2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  1
  48 Am(OH)3(aq)             3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0
  49 Tb++++                  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  4
  50 UO2++                   0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  2
  51 NpO2OH(aged)_______     1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
  52 NpO2OH(amor)_______     1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
  53 NaNpO2CO3(s)_______     0  5  1  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  1  0  0  0  0  0
  54 Na3NpO2(CO3)2(s)_DI     0  8  3  0  0  0  0  0  0  2  0  0  0  0  0  0  0  0  1  0  0  0  0  0
  55 AmOHCO3(c)_______       1  4  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  1  0  0  0  0  0
  56 Am(OH)3(s)_______       3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0
  57 NaAm(CO3)2.6H2O(c)_    12 12  1  0  0  0  0  0  0  2  0  0  0  0  0  0  0  0  1  0  0  0  0  0
  58 AmPO4(c)_____________   0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
  59 CaSO4________________   0  4  0  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  1  0  0  0  1  0
  60 NaK3(SO4)2__Aphthit     0  8  1  3  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  61 CaCl2.6H2O___________  12  6  0  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  62 CaCO3________________   0  3  0  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  63 K2SO4________________   0  4  0  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  64 NgCl2.6H2O___________  12  6  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  65 NaMg(SO4)2.4H2O_____    8 12  2  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  66 Mg(OH)2______________   2  2  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  67 Na6CO3(SO4)2_________   0 11  6  0  0  0  0  2  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  68 CaCO3________________   0  3  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  69 CaCl2.4H2O_____CaC      8  4  0  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  70 Ca4Cl2(OH)6.13H2O__    32 19  0  0  0  0  4  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  71 Ca2Cl2(OH)2.H2O_____    4  3  0  0  0  0  2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  72 KMgCl3.6H2O__________  12  6  0  1  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  73 MgSO4.7H2O___________  14 11  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  74 CaNa2(CO3)2.5H2O____   10 11  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  75 Na2Ca(SO4)2__________   0  8  2  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  76 CaSO4.2H2O___________   4  6  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  77 NaCl_________________   0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  78 MgSO4.6H2O___________  12 10  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  79 KMgClSO4.3H2O________   6  7  0  1  1  0  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  80 KHCO3________________   1  3  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  81 MgSO4.H2O____________   2  5  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  82 K2Mg(SO4)2.4H2O_____    8 12  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  83 Na4Ca(SO4)3.2H2O_____   4 14  4  2  0  0  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  84 MgCO3________________   0  3  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  85 Mg2Cl(OH)3.4H2O_____   11  7  0  0  2  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  86 KHSO4________________   1  4  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  87 Na2SO4.10H2O_________  20 14  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  88 K8N6(SO4)7___________   6 28  0  8  0  0  0  7  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  89 NaHCO3_______________   1  3  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  90 Na2CO3.10H2O_________  20 13  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  91 MgCO3.3H2O___________   6  6  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  92 K2Mg(SO4)2.6H2O Pic    12 14  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  93 Na2Ca(CO3)2.2H2O_____   4  6  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  94 K2MgCa2(SO4)4.2H2O_    4 18  0  2  1  2  0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  95 Ca(OH)2______________   2  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  96 K2CO3.3/2H2O___Pota     3  4  0  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  97 K8N4(CO3)6.3H2O___K    10 21  0  8  0  0  0  0  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  98 KNaCO3.6H2O__________  12  9  1  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
  99 K2NaH(CO3)2.2H2O_____   5  8  1  2  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 100 K3H(SO4)2__Sesquipo     1  8  0  3  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 101 NaJH(SO4)2____Sesqu     1  8  3  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 102 Na2CO3.7H2O____Na2C    14 10  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 103 KCl_________________   0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 104 K2Ca(SO4)2.H2O______   2  9  0  2  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 105 Mg2CaCl6.12H2O______  24 12  0  0  2  1  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 106 Na2SO4______________   0  4  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 107 Na2CO3.H2O__________   2  4  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 108 NaJH(CO3)2.2H2O_____   5  8  3  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 109 Na2B4O7.10H2O_______  20 17  2  0  0  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0
 110 B(OH)3_____________B   3  3  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0
 111 KB5O8.4H2O____K-Pen    8 12  0  1  0  0  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0
 112 K2B4O7.4H2O___K-Tet    8 11  0  2  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0  0
 113 NaBO2.4H2O_____Bo      8  6  1  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
 114 NaB5O8.5H2O_____Sod   10 13  1  0  0  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0  0
 115 NaBO2.NaCl.2H2O___T    4  4  2  0  0  0  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0
 ***************************************************************************************************************************************

 RHOMIN    file name is U1:[SCBABB.FMT.UM]FMT_HMM_NP_AM_RTEST.RHOMIN;1
 # inversions for batch pblm          56
 1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
 DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

 Elemental Abundances for Flash Problem

   Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

   1.11017363E+02   1.11029658E+02   1.00100314E+02   1.00891107E+05  Hydrogen
   6.15086815E+01   6.15154934E+01   5.54601388E+01   8.87328944E+05  Oxygen
   5.61000000E+00   5.61062129E+00   5.05833276E+00   1.16289907E+05  Sodium
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
   1.61000000E+00   1.61017830E+00   1.45167838E+00   5.14663538E+04  Chlorine
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
   2.00000001E+00   2.00022150E+00   1.80311719E+00   2.16597629E+04  Carbon
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Posion
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Negion
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Np(V)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
  -1.77635684E-15  -1.77655356E-15  -1.60167629E-15   0.00000000E+00  Charge

   Solution Parameters, Calculated
     SOLUTION MASS      1306.07033809890      grams
     H2O MASS           999.889265717486      grams
     TDS(g/kg)          306.214981877726      g/kgH2O

   Specified Solution Density
     DENSITY            1177.63607439302      kg/m^3 = g/l

   Solution Parameters Based on Specified Density
     SOLUTION VOL       1.10906108219560      liters
     TDS                276.072326670473      g/l

   Density based on TDS and NaCl solutions     1177.63607439302      g/l
   Percent relative error vs NaCl density    0.000000000000000E+000 %
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
363 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
364
365 Species Name                              Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
366
367 H2O                              WATER    8.57664E-01   8.59843E-01    1.003        5.55025E+01   5.00446E+01   9.01564E+05
368 Na+                               Na+     5.61062E+00   3.69881E+00   0.6593        5.61000E+00   5.05833E+00   1.16290E+05
369 CO3=                             CO3=     1.99407E+00   4.09214E-02   2.0522E-02    1.99385E+00   1.79778E+00   1.07884E+05
370 Cl-                               Cl-     1.61018E+00   1.06477E+00   0.6613        1.61000E+00   1.45168E+00   5.14664E+04
371 HCO3-                            HCO3-    6.14734E-03   3.59044E-03   0.2567        6.14666E-03   5.54222E-03   1.38170E+02
372 OH-                               OH-     6.14733E-03   4.86901E-03   0.7921        6.14665E-03   5.54221E-03   9.42580E+01    2.07E-11
373 CO2(aq)                         CO2(aq)   2.36876E-09   7.15913E-09    3.022        2.36850E-09   2.13559E-09   9.39868E-05   -2.10E-07
374 H+                                H+      2.39954E-12   1.77959E-12   0.7416        2.39927E-12   2.16334E-12   2.18043E-09   -8.49E-08
375 HCl(aq).....to.titrate.acid.only          0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+02
376 NaOH(aq).....to.titrate.base.only         0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.92E+02
377 Na2CO3.10H2O_____________Natron           0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -8.30E-02
378 Na2CO3.H2O_____Thermonatrite              0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.99E-01
379 Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.51E-01
380 NaHCO3_____________________Nahcolite      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.83E+00
381 NaCl_______________________Halite         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -9.75E-01
382 Na3H(CO3)2.2H2O_____________Trona         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.57E+00
383
384 pH (-log[aH+]); pmH(-log[mH+])      11.7497      11.6199
385 Osmotic Coefficient=     0.908418
386 Equilibrium RH (%) =    85.984284
387 Ionic Strength (m) =     7.604695
388 Density, kg/m3     =     1177.64
389 fCO2(g); log[fCO2(g)]=                                  2.171E-07    -6.66
390
391 NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
392         - Gas "molality" and "activity" are gas partial pressures
393         - "Descriptor" means:
394           *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
395           *Saturation Index for minerals, SI=log10(IAP/Ksp)
396           *log10(activity) for aqueous species with very small concentrations
397           *log10(partial pressure) for gases
398
399 Total G/RT=     -6.42133776E+03
400
401 Reaction #              1 sidsum    2.00000000000000
402 This is a solid-only reaction
403
404 shifting left by     4.644346544478256
405 calling makenuv for allomorphic reactions
406 # inversions for batch pblm          99
407 1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
408  DATABASE:  NPM04/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
409  95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,PKP90,P91,RFFR92,RFF94,RRFF94)
410       Pressure=     1.00000E+00 [=] ATM      Temperature=     2.98E+02 [=] Kelvin
411
412  Elemental Abundances for Flash Problem
413
414    Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
415
416    1.11018363E+02   1.11017591E+02   9.93838868E+01   1.00169020E+05  Hydrogen
417    1.05508682E+02   5.55113597E+01   4.96942389E+01   7.95078006E+05  Oxygen
418    1.56100000E+01   5.61057382E+00   5.02263316E+00   1.15469181E+05  Sodium
419    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
420    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
421    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
422    5.61100000E+00   5.61096098E+00   5.02297975E+00   1.78079701E+05  Chlorine
423    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
424    1.00000000E+01   6.12839260E-04   5.48618892E-04   6.58946151E+00  Carbon
425    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
426    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
427    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
428    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
429    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
430    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
431    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
432    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
433    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
434    1.00000000E+01   6.12839260E-04   5.48618892E-04   1.30049121E+02  Np(V)
435    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
436    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
437    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
438   -4.28740972E-15  -4.28737990E-15  -3.83809877E-15   0.00000000E+00  Charge
439
440    Solution Parameters, Calculated
441      SOLUTION MASS      1328.11614865108      grams
442      H2O MASS           1000.006954668820     grams
443      TDS(g/kg)          328.106912108174      g/kgH2O
444
445    Specified Solution Density
446      DENSITY            1188.93254605458      kg/m^3 = g/l
447
448    Solution Parameters Based on Specified Density
449      SOLUTION VOL       1.11706602116190      liters
450      TDS                293.724084133903      g/l
451
452    Density based on TDS and NaCl solutions     1188.93254605458      g/l
453    Percent relative error vs NaCl density    0.00000000000000E+000 %
454
455
456
457  TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
458
459  Species Name                              Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
460
461  H2O                              WATER    8.31822E-01   7.77959E-01   0.9352        5.55091E+01   4.96918E+01   8.95208E+05
462  NaNpO2CO3(s)_____________NaNpO2CO3(s)    5.99932E+00   1.00000E+00    1.000        9.99539E+00   8.95147E+00   3.15133E+06
463  Cl-                               Cl-     5.61096E+00   5.29329E+00   0.9434        5.61100E+00   5.02298E+00   1.78080E+05
464  Na+                               Na+     5.61057E+00   5.29268E+00   0.9433        5.61061E+00   5.02263E+00   1.15469E+05
465  NpO2+                           NpO2+     6.12705E-04   1.21978E-03    1.991        6.12709E-04   5.48499E-04   1.47572E+02
466  CO2(aq)                       CO2(aq)     3.86103E-04   1.12115E-03    2.904        3.86106E-04   3.45643E-04   1.52117E+01
467  HCO3-                           HCO3-     2.26571E-04   8.38810E-05   0.3702        2.26573E-04   2.02829E-04   1.23760E+01    1.23E-14
468  H+                                H+      1.21872E-06   4.78095E-06    3.923        1.21873E-06   1.09101E-06   1.09962E-03    1.23E-14
469  NpO2CO3-                     NpO2CO3-     1.33526E-07   2.42971E-07    1.820        1.33527E-07   1.19534E-07   3.93334E-02    1.85E-14
470  CO3=                             CO3=     3.09384E-08   8.03343E-10   2.5966E-02    3.09386E-08   2.76963E-08   1.66203E-03    0.00E+00
471  OH-                               OH-     3.01685E-09   1.63977E-09   0.5435        3.01687E-09   2.70071E-09   4.59318E-05    1.23E-14
472  NpO2OH(aq)                 NpO2OH(aq)     7.72186E-10   7.72186E-10    1.000        7.72191E-10   6.91267E-10   1.97740E-04   -6.17E-15
473  NpO2(CO3)2=-             NpO2(CO3)2=-     1.98384E-11   5.13355E-16   2.5877E-05    1.98385E-11   1.77595E-11   6.90960E-06    0.00E+00
474  NpO2(OH)2-                 NpO2(OH)2-     2.04381E-16   6.10703E-17   0.2988        2.04383E-16   1.82964E-16   5.54494E-11    0.00E+00
475  NpO2(CO3)3=5-            NpO2(CO3)3=5-    1.25197E-16   9.67897E-26   7.8908E-10    1.25198E-16   1.12077E-16   5.03310E-11   -2.25E-09
476  HCl(aq).....to.titrate.acid.only          0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
477  NaOH(aq).....to.titrate.base.only         0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.99E+02
478  NpO2OH(amor)_____________NpO2OH(amor)     0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
479  Na3H(CO3)2.2H2O_____________Trona         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
480  Na2CO3.H2O_____Thermonatrite              0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
481  Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
482  Na2CO3.10H2O_____________Natron           0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
483  NaHCO3_____________________Nahcolite      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
484  NaCl_______________________Halite         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
485  Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
486  NpO2OH(aged)_____________NpO2OH(aged)     0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
pH (-log[aH+]); pmH(-log[mH+])      5.3205       5.9141
Osmotic Coefficient=     1.341871
Equilibrium RH (%) =    77.795863
Ionic Strength (m) =     5.611188
Density, kg/m3     =     1188.93
fCO2(g); log[fCO2(g)]=                                  3.400E-02    -1.47

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -1.33323084E+04
Flushing Titration #          1
# inversions for batch pblm          17
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
 DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM     Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

  3.85857174E+01   1.11017591E+02   9.93838868E+01   1.00169020E+05  Hydrogen
  3.66707638E+01   5.55113597E+01   4.96942389E+01   7.95078006E+04  Oxygen
  5.42543623E+00   5.61057382E+00   5.02263316E+00   1.15469181E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95016801E+00   5.61096098E+00   5.02297975E+00   1.78079701E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47561578E+00   6.12839260E-04   5.48618892E-04   6.58946151E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   6.12839260E-04   5.48618892E-04   1.30049121E+02  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.94659251E-15  -5.60067366E-15  -5.01377045E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      461.602144251003      grams
    H2O MASS           347.563995068949      grams
    TDS(g/kg)          328.106912108174      g/kgH2O

  Specified Solution Density
    DENSITY            1188.93254605458      Kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.388249228926239       liters
    TDS              293.724084133903        g/l

  Density based on TDS and NaCl solutions     1188.93256605458      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                  WATER  8.31822E-01   7.77959E-01   0.9352        1.92928E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.99932E+00   1.00000E+00   1.000         3.47540E+00   8.95147E+00   3.15133E+06
Cl-                                  Cl-    5.61096E+00   5.29329E+00   0.9434        1.95017E+00   5.02298E+00   1.78080E+05
Na+                                  Na+    5.61057E+00   5.29288E+00   0.9433        1.95003E+00   5.02263E+00   1.15469E+05
NpO2+                              NpO2+    6.12705E-04   1.21978E-03   1.991         2.12954E-04   5.48499E-04   1.47572E+02
CO2(aq)                          CO2(aq)    3.86103E-04   1.12115E-03   2.904         1.34196E-04   3.45643E-04   1.52117E+01
HCO3-                              HCO3-    2.26571E-04   8.38810E-05   0.3702        7.87481E-05   2.02829E-04   1.23760E+01   -5.15E-12
H+                                   H+     1.21872E-06   4.78095E-06   3.923         4.23582E-07   1.09101E-06   1.09962E-03   -2.29E-11
NpO2CO3-                        NpO2CO3-    1.33526E-07   2.42971E-07   1.820         4.64090E-08   1.19534E-07   3.93334E-02    1.85E-14
CO3=                               CO3=     3.09384E-08   8.03343E-10   2.5966E-02    1.07531E-08   2.76963E-08   1.66203E-03    1.68E-11
OH-                                 OH-     3.01685E-09   1.63977E-09   0.5435        1.04855E-09   2.70071E-09   4.59118E-05    2.30E-11
NpO2OH(aq)                    NpO2OH(aq)    7.72186E-10   7.72186E-10   1.000         2.68384E-10   6.91267E-10   1.97740E-04    6.15E-12
NpO2(CO3)2=-                NpO2(CO3)2=-    1.98384E-11   5.13355E-16   2.5877E-05    6.89511E-12   1.77595E-11   6.90960E-06    1.69E-11
NpO2(OH)2-                    NpO2(OH)2-    2.04381E-16   6.10703E-17   0.2988        7.10356E-17   1.82964E-16   5.54494E-11    2.92E-11
NpO2(CO3)3=-                NpO2(CO3)3=-    1.25197E-16   9.87897E-26   7.8908E-10    4.35139E-17   1.12077E-16   5.03310E-11   -3.15E-10
HCl(aq).....to.titrate.acid.only            0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
NaOH(aq).....to.titrate.base.only           0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.99E+02
NaJH(CO3)2.2H2O_____________Trona           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
Na2CO3.H2O_____Thermonatrite                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.10H2O_____________Natron             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
NaHCO3_____________Nahcolite                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
NaCl_____________Halite                     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NpO2OH(amor)_____________NpO2OH(amor)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
NpO2OH(aged)_____________NpO2OH(aged)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00

pH (-log[aH+]); pmH(-log[mH+])      5.3205       5.9141
Osmotic Coefficient=     1.341871
Equilibrium RH (%) =    77.795863
Ionic Strength (m) =     5.611188
Density, kg/m3     =     1188.93
fCO2(g); log[fCO2(g)]=                                  3.400E-02    -1.47

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.63379813E+03
Flushing Titration #          2
# inversions for batch pblm          19
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
 DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM     Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.85957275E+01	1.11017746E+02	9.93891116E+01	1.00174286E+05	Hydrogen
3.66761098E+01	5.55107903E+01	4.96962723E+01	7.95110540E+05	Oxygen
5.42594206E+00	5.61041055E+00	5.02250276E+00	1.15466183E+05	Sodium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1.95031318E+00	5.60993114E+00	5.02231483E+00	1.78056128E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47579611E+00	6.90933317E-04	6.18560128E-04	7.42952570E+00	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Poslon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neglon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
3.47561578E+00	1.72218651E-04	1.54179484E-04	1.65479691E+01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4-(EL)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
-1.36269746E-15	-3.91969811E-15	-3.50912649E-15	0.00000000E+00	Charge

Solution Parameters, Calculated

SOLUTION MASS	461.665999617212	grams
H2O MASS	347.653675949709	grams
TDS(g/kg)	327.947988724245	g/kgH2O

Specified Solution Density

DENSITY	1188.85111178691	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	0.388329534508861	liters
TDS	293.596838859294	g/l

Density based on TDS and NaCl solutions 1188.85111178691 g/l
Percent relative error vs NaCl density 0.000000000000000E+000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31845E-01	7.78011E-01	0.9353	1.92978E+01	4.96944E+01	8.95254E+05	
NaNpO2CO3(s)	NaNpO2CO3(s)	9.99718E+00	1.00000E+00	1.000	3.47556E+00	8.95002E+00	3.15082E+06	
Na+	Na+	5.61014E+00	5.29140E+00	0.9432	1.95039E+00	5.02250E+00	1.15466E+05	
Cl-	Cl-	5.60993E+00	5.29139E+00	0.9432	1.95031E+00	5.02231E+00	1.78056E+05	
HCO3-	HCO3-	3.82212E-04	1.41513E-04	0.3702	1.32878E-04	3.42177E-04	2.08787E+01	
CO2(aq)	CO2(aq)	3.08476E-04	8.95671E-04	2.904	1.07243E-04	2.76165E-04	1.21539E+01	
NpO2+	NpO2+	1.72085E-04	3.42481E-04	1.990	5.98258E-05	1.54059E-04	4.14492E+01	-1.82E-10
H+	H+	5.77346E-07	2.26410E-06	3.922	2.00716E-07	5.16872E-07	5.20955E-04	-2.18E-10
NpO2CO3-	NpO2CO3-	1.33573E-07	2.43030E-07	1.819	4.64370E-08	1.19581E-07	3.93490E-02	8.02E-14
CO3=	CO3=	1.10196E-07	2.86188E-09	2.5971E-02	3.83099E-08	9.86531E-08	5.92010E-03	3.31E-10
OH-	OH-	6.37029E-09	3.46282E-09	0.5436	2.21466E-09	5.70303E-09	9.69932E-05	2.19E-10
NpO2OH(aq)	NpO2OH(aq)	4.57851E-10	4.57851E-10	1.000	1.59174E-10	4.09893E-10	1.17252E-04	-1.14E-10
NpO2(CO3)2=-	NpO2(CO3)2=-	7.06677E-11	1.82925E-15	2.5885E-05	2.45679E-11	6.32656E-11	2.46144E-05	1.32E-10
NpO2(CO3)3===	NpO2(CO3)3==	1.58546E-15	1.25406E-24	7.9097E-10	5.51192E-16	1.41939E-15	6.37413E-10	5.26E-10
NpO2(OH)2-	NpO2(OH)2-	2.55903E-16	7.66679E-17	0.2988	8.89657E-17	2.29098E-16	6.94309E-11	1.05E-10
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.45E+02
NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+02
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.61E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.21E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.36E+02
NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.72E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.36E+00
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.40E+00
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.69E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.40E+00

pH (-log[aH+]); pmH(-log[mH+]) 5.6451 6.2386
Osmotic Coefficient= 1.241740
Equilibrium RH (%) = 77.801108
Ionic Strength (m) = 5.610314
Density, kg/m3 = 1188.85
fCO2(g); log[fCO2(g)]= 2.716E-02 -1.57

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
"dG/RT/ln10 for species with nonzero concs. (convergence criterion)
"Saturation Index for minerals, SI=log10(IAP/Ksp)
"log10(activity) for aqueous species with very small concentrations
"log10(partial pressure) for gases

Total G/RT= -8.63438031E+03
Flashing Titration # 3
inversions for batch phlm 20
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.6Imolal NaCl FMT V2.1
DATABASE: NMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31 Am(III)-Na-Cl-CO3-EO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFT94,RFFT94)
Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.86057375E+01	1.11018354E+02	9.93915377E+01	1.00176731E+05	Hydrogen
3.66818559E+01	5.55117917E+01	4.96981098E+01	7.95139938E+05	Oxygen
5.42644790E+00	5.61000017E+00	5.02247173E+00	1.15465470E+05	Sodium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1.95045835E+00	5.60892471E+00	5.02150891E+00	1.78027555E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47597644E+00	1.03777160E-03	9.29087049E-04	1.11592645E+01	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Poslon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neglon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
3.47561578E+00	6.07539648E-07	5.43912238E-07	1.28933415E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4-(EL)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
 -1.62342993E-15  -4.66849050E-15  -4.17956521E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS        461.762759746566        grams
   H2O MASS             347.741937885849        grams
   TDS(g/kg)            327.889188614766        g/kgH2O

 Specified Solution Density
   DENSITY              1188.82098252588        kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL      0.3884207685882?1          liters
   TDS                  293.549756961959        g/l

 Density based on TDS and NaCl solutions     1188.82098252588       g/l
 Percent relative error vs NaCl density     0.0000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                 WATER   8.31857E-01   7.78049E-01   0.9353        1.93027E+01   4.96953E+01   8.95271E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.99481E+00   1.00000E+00   1.000         3.47562E+00   8.94607E+00   3.15013E+06
Na+                                 Na+     5.61000E+00   5.29001E+00   0.9430        1.95083E+00   5.02247E+00   1.15465E+05
Cl-                                 Cl-     5.60892E+00   5.29003E+00   0.9431        1.95046E+00   5.02151E+00   1.78028E+05
HCO3-                               HCO3-   9.89705E-04   3.66450E-04   0.3703        3.44162E-04   8.86055E-04   5.40645E+01
CO3=                                CO3=    4.25167E-05   1.10426E-06   2.5972E-02    1.47848E-05   3.80640E-05   2.28619E+00
CO2(aq)                             CO2(aq) 5.36072E-06   1.55648E-05   2.903         1.86415E-06   4.79930E-06   2.11216E-01   -3.58E-08
OH-                                 OH-     9.49137E-07   5.16005E-07   0.5437        3.30055E-07   8.49735E-07   1.44517E-02   -1.27E-07
NpO2+                               NpO2+   4.46247E-07   8.87829E-07   1.990         1.55179E-07   3.99512E-07   1.07407E-01    2.08E-07
NpO2CO3-                            NpO2CO3-1.33612E-07   2.43093E-07   1.819         4.64625E-08   1.19619E-07   3.93614E-02   6.11E-13
NpO2(CO3)2=-                        NpO2(CO3)2=-2.72677E-08   7.06005E-13   2.5892E-05    9.48211E-09   2.44120E-08   9.49785E-03   -1.46E-07
H+                                  H+      3.87609E-09   1.51947E-08   3.920         1.34788E-09   3.47015E-09   3.49756E-06    1.59E-07
NpO2(CO3)3=5-                       NpO2(CO3)3=5-2.35800E-10   1.86755E-19   7.9201E-10    8.19976E-11   2.11105E-10   9.48020E-05   -2.85E-07
NpO2OH(aq)                          NpO2OH(aq) 1.76865E-10   1.76865E-10   1.000         6.15033E-11   1.58342E-10   4.52944E-05   -1.72E-08
NpO2(OH)2-                          NpO2(OH)2-1.47303E-14   4.40176E-15   0.2988        5.12234E-15   1.31876E-14   3.99666E-09   -1.77E-07
HCl(aq).....to.titrate.acid.only    0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.47E-02
NaOH(aq).....to.titrate.base.only   0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.96E-02
NpO2OH(aged)_____________NpO2OH(aged)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.02E+00
NpO2OH(amor)_____________NpO2OH(amor)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.62E+00
NaJNpO2(CO3)2(s)_DISABLED_DISABLED          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.33E+02
NaCl_____________________________Halite     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3___________________________Nahcolite  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.31E+00
Na2CO3.10H2O_____________________Natron     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.78E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.81E+00
Na2CO3.H2O_______Thermonatrite              0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -5.10E+00
Na3H(CO3)2.2H2O__________Trona              0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -6.40E+00

pH (-log[aH+]); pmH(-log[mH+])      7.0183        8.4116
Osmotic Coefficient=    1.241604
Equilibrium RH (%) =   77.804942
Ionic Strength (m) =    5.610043
Density, kg/m3     =    1188.82
fCO2(g); log[fCO2(g)]=                                    4.720E-04    -3.33

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.63496201E+03
Flashing Titration #          4
# inversions for batch pbln          22
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFK92,RFP94,RRFP94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.86157475E+01   1.11018385E+02   9.93917354E+01   1.00176930E+05  Hydrogen
  3.66874019E+01   5.55133618E+01   4.96996003E+01   7.95163785E+05  Oxygen
  5.42695373E+00   5.61000172E+00   5.02248168E+00   1.15465699E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95060352E+00   5.60788970E+00   5.02059085E+00   1.77995007E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47615678E+00   1.55589938E-03   1.39295432E-03   1.67107744E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   5.56117383E-07   4.97894645E-07   1.18025010E-01  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.42050632E-15  -4.08188619E-15  -3.65619203E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS        461.880517078989        grams
   H2O MASS             347.812004756083        grams
   TDS(g/kg)            327.883894418751        g/kgH2O

 Specified Solution Density
   DENSITY              1188.81826953613        kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL      0.388520709106543          liters
   TDS                  293.545516750385        g/l

 Density based on TDS and NaCl solutions     1188.81826953613       g/l
 Percent relative error vs NaCl density     0.0000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                 WATER   8.31863E-01   7.78070E-01   0.9353        1.93077E+01   4.96954E+01   8.95273E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.99222E+00   1.00000E+00   1.000         3.47562E+00   8.94577E+00   3.14932E+06
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

Na+	Na+	5.61000E+00	5.28968E+00	0.9429	1.95134E+00	5.02248E+00	1.15466E+05	
Cl-	Cl-	5.60789E+00	5.28851E+00	0.9430	1.95060E+00	5.02059E+00	1.77995E+05	
HCO3-	HCO3-	1.01025E-03	3.74021E-04	0.3702	3.51398E-04	9.04652E-04	5.51870E+01	
CO3=	CO3=	5.44263E-04	1.41351E-05	2.5971E-02	1.89312E-04	4.87264E-04	2.92603E+01	
OH-	OH-	1.19027E-05	6.47157E-06	0.5437	4.14015E-06	1.06562E-05	1.81233E-01	-6.88E-08
CO2(aq)	CO2(aq)	4.36260E-07	1.26669E-06	2.904	1.51745E-07	3.90571E-07	1.71890E-02	-1.17E-07
NpO2(CO3)2=	NpO2(CO3)2=	3.48678E-07	9.03777E-12	2.5905E-05	1.21351E-07	3.12341E-07	1.31521E-01	3.10E-08
NpO2CO3-	NpO2CO3-	1.13632E-07	2.43109E-07	1.619	4.64814E-08	1.19637E-07	3.93673E-02	5.65E-12
NpO2(CO3)3=3-	NpO2(CO3)3=3-	3.85776E-08	3.06022E-17	7.9326E-10	1.34185E-08	3.45174E-08	1.55099E-02	5.13E-08
NpO2+	NpO2+	3.48770E-08	6.93635E-08	1.989	1.21313E-08	3.12244E-08	8.40081E-03	-2.34E-08
H+	H+	3.09280ZE-10	1.21157E-09	3.918	1.07550E-10	2.76820E-10	2.79007E-07	-2.81E-08
NpO2OH(aq)	NpO2OH(aq)	1.73100E-10	1.73100E-10	1.000	6.02793E-11	1.55151E-10	4.43815E-05	5.12E-09
NpO2(OH)2-	NpO2(OH)2-	1.81034E-13	5.40520E-14	0.2988	6.29695E-14	1.62075E-13	4.91167E-08	3.23E-08
HCl(aq) .....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
NaOH(aq) .....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.63E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.32E+02
NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.38E+00
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.42E+00
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.71E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.99E+00

pH (-log[aH+]); pmH(-log[mH+]) 8.9167 9.5698
Osmotic Coefficient= 1.241531
Equilibrium RH (%) = 77.806961
Ionic Strength (m) = 5.610547
Density, kg/m3 = 1188.82
fCO2(g): log[fCO2(g)]= 3.841E-05 -4.42

NOTES: + Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -4.63554267E+01
Flashing Titration # 5
inversions for batch pblm 23
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.6lmolal NaCl FMT V2.3
DATABASE: YMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (RR94);
95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRER89,FRF90,P91,RFFR92,RFF94,RRFF94)
Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1.86257575E+01	1.11016407E+02	9.93919228E+01	1.00177119E-05	Hydrogen
3.66929479E+01	5.55149287E+01	4.97010869E+01	7.95187570E+05	Oxygen
5.42745956E+00	5.61000325E+00	5.02249153E+00	1.15465925E+05	Sodium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1.95074868E+00	5.60685474E+00	5.01967275E+00	1.77962458E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47633711E+00	2.07422268E-01	1.85699819E-01	2.23044052E+01	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Fusion
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neglon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Tb(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
3.47561578E+00	9.68717529E-07	8.67267874E-07	2.05584288E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4-(EL)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
-1.86173167E-15	-5.35100145E-15	-4.79061389E-15	0.00000000E+00	Charge

Solution Parameters, Calculated
SOLUTION MASS 461.998331238771 grams
H2O MASS 347.922101921007 grams
TDS(g/kg) 327.878650674697 g/kgH2O

Specified Solution Density
DENSITY 1188.81558239116 kg/m^3 = g/l

Solution Parameters Based on Specified Density
SOLUTION VOL 0.388620689414030 liters
TDS 293.541317843627 g/l

Density based on TDS and NaCl solutions 1188.81558239116 g/l
Percent relative error vs NaCl density 0.000000000000000E+000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31869E-01	7.78090E-01	0.9354	1.93127E+01	4.96955E+01	8.95274E+05	
NaNpO2CO3(s)	NaNpO2CO3(s)	9.98964E+00	1.00000E+00	1.000	3.47562E+00	8.94346E+00	3.14851E+06	
Na+	Na+	5.61000E+00	5.28936E+00	0.9428	1.95134E+00	5.02249E+00	1.15466E+05	
Cl-	Cl-	5.60685E+00	5.28698E+00	0.9429	1.95075E+00	5.01967E+00	1.77962E+05	
CO3=	CO3=	1.05085E-03	2.72900E-05	2.5970E-02	3.65612E-04	9.40794E-04	5.64563E+01	
HCO3-	HCO3-	1.02124E-03	3.78050E-04	0.3702	3.55311E-04	9.14286E-04	5.57871E+01	
OH-	OH-	2.27338E-05	1.23615E-05	0.5438	7.90961E-06	2.03530E-05	3.46150E-01	-3.63E-09
NpO2(CO3)2=-	NpO2(CO3)2=-	6.73247E-07	1.74499E-11	2.5919E-05	2.34230E-07	6.02741E-07	2.34506E-01	8.77E-09
CO2(aq)	CO2(aq)	2.30850E-07	6.70283E-07	2.904	8.03179E-08	2.06674E-07	9.09569E-03	-2.99E-08
NpO2(CO3)3=5-	NpO2(CO3)3=5-	1.43575E-07	1.14074E-16	7.9453E-10	4.99528E-08	1.28539E-07	5.77235E-02	1.73E-08
NpO2CO3-	NpO2CO3-	1.33651E-07	2.43123E-07	1.819	4.65003E-08	1.19655E-07	3.93731E-02	1.47E-12
NpO2+	NpO2+	1.80727E-08	3.59296E-08	1.988	6.28788E-09	1.61800E-08	4.35318E-03	-8.17E-09
NpO2OH(aq)	NpO2OH(aq)	1.71468E-10	1.71468E-10	1.000	5.96575E-11	1.53511E-10	4.39124E-05	8.75E-09
H+	H+	1.61951E-10	6.34304E-10	3.917	5.63465E-11	1.44991E-10	1.46136E-07	-1.69E-08
NpO2(OH)2-	NpO2(OH)2-	3.42173E-13	1.02231E-13	0.2988	1.19050E-13	3.06339E-13	9.28396E-08	2.56E-08
HCl(aq) .....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.49E+02
NaOH(aq) .....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.04E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.63E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.32E+02
NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.38E+00
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.42E+00
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.71E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.99E+00

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
pH (-log[aH+]); pmH(-log[mH+])        9.1977        9.7906
Osmotic Coefficient=     1.241460
Equilibrium RH (%) =    77.808967
Ionic Strength (m) =     5.611058
Density, kg/m3     =     1188.82
fCO2(g); log[fCO2(g)]=                                    2.033E-05    -4.69

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -4.63612311E+03
Flashing Titration #            6
# inversions for batch pblm           23
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.6lmolal NaCl  FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.86357676E+01  1.11018428E+02  9.93921088E+01  1.00177306E+05  Hydrogen
  3.66984939E+01  5.55164947E+01  4.97025726E+01  7.95211340E+05  Oxygen
  5.42796540E+00  5.61000482E+00  5.02250138E+00  1.15466152E+05  Sodium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
  1.95089385E+00  5.60582027E+00  5.01875506E+00  1.77929923E+05  Chlorine
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
  3.47651744E+00  2.59235463E-03  2.32087229E-03  2.78759970E-01  Carbon
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  PosIon
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  NegIon
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Th(IV)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
  3.47561578E+00  1.45812117E-06  1.30542055E-06  3.09447592E-01  Np(V)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  ClO4-(EL)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electron
 -1.42171696E-15 -4.08525032E-15 -3.65742562E-15  0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      462.116154836857      grams
    H2O MASS           348.012201242052      grams
    TDS(g/kg)          327.873428539486      g/kgH2O

  Specified Solution Density
    DENSITY            1188.81290631058      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.388720674534911       liters
    TDS               293.537136225970       g/l

  Density based on TDS and NaCl solutions     1188.81290631058      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                WATER    8.31876E-01   7.78110E-01   0.9354        1.93177E+01   4.96956E+01   8.95276E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.98705E+00   1.00000E+00    1.000        3.47562E+00   8.94116E+00   3.14770E+06
Na+                                Na+      5.61000E+00   5.28904E+00   0.9428        1.95235E+00   5.02250E+00   1.15466E+05
Cl-                                Cl-      5.60582E+00   5.28565E+00   0.9429        1.95089E+00   5.01876E+00   1.77930E+05
CO3=                              CO3=      1.55739E-03   4.04423E-05   2.5968E-02    5.41990E-04   1.39429E-03   8.36703E+01
HCO3-                             HCO3-     1.03174E-03   3.81899E-04   0.3702        3.59057E-04   9.23688E-04   5.63600E+01
OH-                                OH-      3.33488E-05   1.81350E-05   0.5438        1.16058E-05   2.98564E-05   5.07777E-01  -1.99E-08
NpO2(CO3)2=-                 NpO2(CO3)2=-    9.97249E-07   2.58614E-11   2.5933E-05    3.47055E-07   8.92813E-07   3.47363E-01   1.99E-08
NpO2(CO3)3=5-                NpO2(CO3)3=5-   3.14830E-07   2.50542E-16   7.9580E-10    1.09565E-07   2.81860E-07   1.26576E-01   4.15E-08
CO2(aq)                          CO2(aq)     1.58957E-07   4.61541E-07   2.904         5.53190E-08   1.42310E-07   6.26305E-03  -1.04E-07
NpO2CO3-                       NpO2CO3-      1.33671E-07   2.43138E-07   1.819         4.65191E-08   1.19672E-07   3.93789E-02   1.02E-12
NpO2+                            NpO2+       1.22005E-08   2.42463E-08   1.987         4.24592E-09   1.09228E-08   2.93875E-03  -1.66E-08
NpO2OH(aq)                   NpO2OH(aq)      1.69754E-10   1.69754E-10   1.000         5.90766E-11   1.51977E-10   4.34737E-05   3.26E-08
H+                                 H+        1.10445E-10   4.32378E-10   3.915,        1.84361E-11   9.88785E-11   9.96596E-08  -4.95E-08
NpO2(OH)2-                   NpO2(OH)2-      4.97012E-13   1.48479E-13   0.2987        1.72966E-13   4.44963E-13   1.34851E-07   8.14E-08
HCl(aq).....to.titrate.acid.only           0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -2.49E+02
NaOH(aq).....to.titrate.base.only          0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -2.95E+02
NpO2OH(aged)_____________NpO2OH(aged)      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -3.04E+00
NpO2OH(amor)_____________NpO2OH(amor)      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -3.64E+00
Na3Np02(CO3)2(s)_DISABLED_DISABLED         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -9.31E+03
NaCl_____________________________Halite    0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -1.24E-01
NaHCO3___________________________Nahcolite  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -2.29E+00
Na2CO3.10H2O_____________________Natron     0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -3.21E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -3.25E+00
Na2CO3.H2O_____________Thermonatrite       0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -3.54E+00
Na3H(CO3)2.2H2O_________________Trona      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -4.61E+00

pH (-log[aH+]); pmH(-log[mH+])        9.3641        9.9569
Osmotic Coefficient=     1.241388
Equilibrium RH (%) =    77.810972
Ionic Strength (m) =     5.611568
Density, kg/m3     =     1188.81
fCO2(g); log[fCO2(g)]=                                    1.400E-05    -4.85

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -4.63670347E+03
Flashing Titration #            7
# inversions for batch pblm           23
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.6lmolal NaCl  FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

	Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
	3.86457776E+01	1.11018449E+02	9.93922937E+01	1.00177493E+05	Hydrogen
	3.67040399E+01	5.55180601E+01	4.97040572E+01	7.95235093E+05	Oxygen
	5.42847123E+00	5.61000643E+00	5.02251124E+00	1.15466378E+05	Sodium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
	1.95103902E+00	5.60478632E+00	5.01783779E+00	1.77897403E+05	Chlorine
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
	3.47669778E+00	3.11028689E-03	2.78456916E-03	3.34454601E+01	Carbon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
	3.47561578E+00	2.01581777E-06	1.80471583E-06	4.27804639E-01	Np(V)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Cl04-(EL)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
	-1.59539651E-15	-4.58112542E-15	-4.10316801E-15	0.00000000E+00	Charge

Solution Parameters, Calculated

SOLUTION MASS	462.233986835158	grams
H2O MASS	348.102302060915	grams
TDS(g/kg)	327.868227601747	g/kgH2O

Specified Solution Density

DENSITY	1188.81024108369	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	0.388820663602122	liters
TDS	293.532971568181	g/l

Density based on TDS and NaCl solutions 1188.81024108369 g/l
Percent relative error vs NaCl density 0.000000000000000E+000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31882E-01	7.78130E-01	0.9354	1.93227E+01	4.96957E+01	8.95277E+05	
NaNpO2CO3(s)	NaNpO2CO3(s)	9.98446E+00	1.00000E+00	1.000	3.47562E+00	8.93686E+00	3.14689E+06	
Na+	Na+	5.61001E+00	5.28872E+00	0.9427	1.95286E+00	5.02251E+00	1.15466E+05	
Cl-	Cl-	5.60479E+00	5.28392E+00	0.9428	1.95104E+00	5.01784E+00	1.77897E+05	
CO3+	CO3+	2.06377E-03	5.35891E-05	2.5967E-02	7.18404E-04	1.84765E-03	1.10876E+02	
HCO3-	HCO3-	1.04196E-03	3.85644E-04	0.3701	3.62709E-04	9.32843E-04	5.69194E+01	
OH-	OH-	4.37579E-05	2.37975E-05	0.5438	1.52322E-05	3.91755E-05	6.66269E-01	-7.34E-08
NpO2(CO3)2e-	NpO2(CO3)2e-	1.32081E-06	3.42703E-11	2.5946E-05	4.59777E-07	1.18249E-06	4.60066E-01	5.47E-08
NpO2(CO3)3e--	NpO2(CO3)3e--	5.51937E-07	4.39934E-16	7.9707E-10	1.92131E-07	4.94137E-07	2.21904E-01	1.21E-07
NpO2CO3-	NpO2CO3-	1.33690E-07	2.43152E-07	1.819	4.65379E-08	1.19690E-07	3.93847E-02	2.67E-12
CO2(aq)	CO2(aq)	1.22321E-07	3.55172E-07	2.904	4.25802E-08	1.09511E-07	4.81956E-03	-4.08E-07
NpO2+	NpO2+	9.21138E-09	1.82991E-08	1.987	3.20650E-09	8.24674E-09	3.21876E-03	-4.64E-08
NpO2OH(aq)	NpO2OH(aq)	1.68120E-10	1.68120E-10	1.000	5.85229E-11	1.50514E-10	4.30552E-05	1.20E-07
H+	H+	8.42049E-11	3.29505E-10	3.913	2.93119E-11	7.53867E-11	7.59823E-08	-1.70E-07
NpO2(OH)2-	NpO2(OH)2-	6.45975E-13	1.92964E-13	0.2987	2.24866E-13	5.78327E-13	1.75269E-07	2.82E-07
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.49E+02
NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.94E+02
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.05E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.64E+00
Na3NpO2(CO3)2(s)	DISABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.31E+02
NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.29E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.09E+00
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.13E+00
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.42E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.69E+00

pH (-log[aH+]); pmH(-log[mH+]) 9.4821 10.0747
Osmotic Coefficient= 1.241316
Equilibrium RH (%) = 77.812976
Ionic Strength (m) = 5.612080
Density, kg/m3 = 1188.81
fCO2(g); log[fCO2(g)]= 1.077E-05 -4.97

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
"dG/RT/ln10 for species with nonzero concs. (convergence criterion)
"Saturation Index for minerals, SI=log10(IAP/Ksp)
"log10(activity) for aqueous species with very small concentrations
"log10(partial pressure) for gases

Total G/RT= -4.63728377E+03
Flashing Titration # 8
inversions for batch pblm 26
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
DATABASE: HMW84/PM85; Np(V)-Na-CO3-OH-Cl-ClO4 (HR94);
95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FMP90,P91,RFFR92,RFF94,RRFF94)
Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

	Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
	3.86557876E+01	1.11018469E+02	9.93924776E+01	1.00177678E+05	Hydrogen
	3.67095859E+01	5.55196248E+01	4.97055410E+01	7.95258832E+05	Oxygen
	5.42897706E+00	5.61000809E+00	5.02252110E+00	1.15466605E+05	Sodium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
	1.95118419E+00	5.60375288E+00	5.01692095E+00	1.77864898E+05	Chlorine
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
	3.47687811E+00	3.62801754E-03	3.24808705E-03	3.90127736E+01	Carbon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
	3.47561578E+00	2.61966944E-06	2.36323959E-06	5.60201786E-01	Np(V)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Cl04-(EL)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
	-7.64533209E-16	-2.19572053E-15	-1.96578196E-15	0.00000000E+00	Charge

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
1231
1232   Solution Parameters, Calculated
1233     SOLUTION MASS      462.351826978109      grams
1234     H2O MASS           348.192404119958      grams
1235     TDS(g/kg)          327.863047864827      g/kgH2O
1236
1237   Specified Solution Density
1238     DENSITY            1188.80758671231      kg/m^3 = g/l
1239
1240   Solution Parameters Based on Specified Density
1241     SOLUTION VOL     0.388920656417378       liters
1242     TDS              293.528823873111        g/l
1243
1244   Density based on TDS and NaCl solutions     1188.80758671231      g/l
1245   Percent relative error vs NaCl density    0.000000000000000E+000 %
1246
1247
1248
1249 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1250
1251 Species Name                          Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
1252
1253 H2O                          WATER    8.31888E-01   7.78150E-01   0.9354        1.93277E+01   4.96957E+01   8.95279E+05
1254 NaNpO2CO3(s)_____NaNpO2CO3(s)        9.98188E+00   1.00000E+00   1.000         3.47561E+00   8.93657E+00   3.14608E+06
1255 Na+                          Na+      5.61001E+00   5.28841E+00   0.9427        1.95336E+00   5.02252E+00   1.15467E+05
1256 Cl-                          Cl-      5.60375E+00   5.28239E+00   0.9427        1.95118E+00   5.01692E+00   1.77865E+05
1257 CO3=                         CO3=     2.56997E-03   6.67295E-05   2.5965E-02    8.94845E-04   2.30084E-03   1.38072E+02
1258 HCO3-                        HCO3-    1.05196E-03   3.89306E-04   0.3701        3.66285E-04   9.41798E-04   5.74658E+01
1259 OH-                          OH-      5.39719E-05   2.93547E-05   0.5439        1.87926E-05   4.83199E-05   8.21791E-01   -4.00E-09
1260 NpO2(CO3)2=-                 NpO2(CO3)2=-   1.64391E-06   4.26761E-11   2.5960E-05   5.72396E-07   1.47176E-06   5.72609E-01   1.61E-08
1261 NpO2(CO3)3=5-                NpO2(CO3)3=5-  8.54484E-07   6.82175E-16   7.9835E-10   2.97525E-07   7.65001E-07   3.43543E-01   3.23E-08
1262 NpO2CO3-                     NpO2CO3-   1.33710E-07   2.43167E-07   1.819         4.65568E-08   1.19708E-07   3.93906E-02   7.97E-12
1263 CO2(aq)                      CO2(aq)    1.00104E-07   2.90667E-07   2.904         3.48556E-08   8.96214E-08   3.94422E-03   -8.97E-08
1264 NpO2+                        NpO2+      7.40067E-09   1.46965E-08   1.986         2.57686E-09   6.62567E-09   1.78262E-03   -1.60E-08
1265 NpO2OH(aq)                   NpO2OH(aq) 1.66553E-10   1.66553E-10   1.000         5.79923E-11   1.49111E-10   4.26538E-05   3.82E-08
1266 H+                           H+         6.82959E-11   2.67131E-10   3.911         2.37801E-11   6.11438E-11   6.16269E-08   -5.42E-08
1267 NpO2(OH)2-                   NpO2(OH)2- 7.89467E-13   2.35806E-13   0.2987        2.74886E-13   7.06793E-13   2.14202E-07   9.25E-08
1268 HCl(aq).....to.titrate.acid.only     0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
1269 NaOH(aq).....to.titrate.base.only    0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
1270 NpO2OH(aged)_____NpO2OH(aged)        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.05E+00
1271 NpO2OH(amor)_____NpO2OH(amor)        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.64E+00
1272 Na3NpO2(CO3)2(s)_DISABLED_DISABLED   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+02
1273 NaCl_____Halite                      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
1274 NaHCO3_____Nahcolite                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.28E+00
1275 Na2CO3.10H2O_____Natron              0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.99E+00
1276 Na2CO3.7H2O____Na2CO3-Heptahydrate   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.03E+00
1277 Na2CO3.H2O_____Thermonatrite         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.32E+00
1278 Na3H(CO3)2.2H2O_____Trona            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.59E+00
1279
1280 pH (-log[aH+]); pmH(-log[mH+])       9.5733        10.1656
1281 Osmotic Coefficient=     1.241245
1282 Equilibrium RH (%) =    77.814978
1283 Ionic Strength (m) =     5.612592
1284 Density, kg/m3     =     1188.81
1285 fCO2(g); log(fCO2(g))=                                 8.815E-06     -5.05
1286
1287 NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
1288         - Gas "molality" and "activity" are gas partial pressures
1289         - "Descriptor" means:
1290           "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
1291           "Saturation Index for minerals, SI=log10(IAP/Ksp)
1292           "log10(activity) for aqueous species with very small concentrations
1293           "log10(partial pressure) for gases
1294
1295 Total G/RT=     -4.63786402E+03
1296 Flashing Titration #          9
1297  # inversions for batch pblm          29
1298 1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.6lmolal NaCl  FMT V2.3
1299 DATABASE:  HMW84/PWB6; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1300 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
1301     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin
1302
1303 Elemental Abundances for Flash Problem
1304
1305   Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter
1306
1307   3.86657977E+01    1.11018489E+02    9.93926605E+01    1.00177862E+05  Hydrogen
1308   3.67151319E+01    5.55211888E+01    4.97070238E+01    7.95282556E+05  Oxygen
1309   5.42948290E+00    5.61000979E+00    5.02253097E+00    1.15466832E+05  Sodium
1310   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
1311   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
1312   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
1313   1.95132936E+00    5.60271996E+00    5.01600453E+00    1.77832409E+05  Chlorine
1314   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
1315   3.47705844E+00    4.14554576E-03    3.71142525E-03    4.45779286E+01  Carbon
1316   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  PosIon
1317   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  NegIon
1318   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
1319   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
1320   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
1321   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
1322   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Th(IV)
1323   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
1324   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
1325   3.47561578E+00    3.12866843E-06    2.98009111E-06    7.06425223E-01  Np(V)
1326   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
1327   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
1328   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
1329  -1.15045794E-15   -3.30323204E-15   -2.95731846E-15    0.00000000E+00  Charge
1330
1331   Solution Parameters, Calculated
1332     SOLUTION MASS      462.469675148448      grams
1333     H2O MASS           348.282507371911      grams
1334     TDS(g/kg)          327.857889384617      g/kgH2O
1335
1336   Specified Solution Density
1337     DENSITY            1188.80494322519      kg/m^3 = g/l
1338
1339   Solution Parameters Based on Specified Density
1340     SOLUTION VOL     0.389020652869917       liters
1341     TDS              293.524693185684        g/l
1342
1343   Density based on TDS and NaCl solutions     1188.80494322519      g/l
1344   Percent relative error vs NaCl density    0.000000000000000E+000 %
1345
1346
1347
1348 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1349
1350 Species Name                          Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
1351
1352 H2O                          WATER    8.31895E-01   7.78170E-01   0.9354        1.93327E+01   4.96958E+01   8.95280E+05
1353 NaNpO2CO3(s)_____NaNpO2CO3(s)        9.97930E+00   1.00000E+00   1.000         3.47561E+00   8.93627E+00   3.14527E+06
1354 Na+                          Na+      5.61001E+00   5.28810E+00   0.9426        1.95387E+00   5.02253E+00   1.15467E+05
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
Cl-                                Cl-      5.60272E+00   5.28086E+00   0.9426    1.95133E+00   5.81600E+00   1.77832E+05
CO3=                               CO3=     3.07597E-03   7.98630E-05   2.5964E-02  1.07131E-03   2.75385E-03   1.65256E+02
HCO3-                              HCO3-    1.06176E-03   3.92894E-04   0.3700    3.69793E-04   9.50573E-04   5.80012E+01
OH-                                OH-      6.40010E-05   3.48124E-05   0.5439    2.22904E-05   5.72988E-05   9.74496E-01   -3.83E-10
Np02(CO3)2=-                       Np02(CO3)2=-  1.96653E-06  5.10785E-11  2.5974E-05  6.84909E-07  1.76060E-06  6.84987E-01   2.72E-09
Np02(CO3)3=5-                      Np02(CO3)3=5- 1.22205E-06  9.77185E-16  7.9962E-10  4.25620E-07  1.09408E-06  4.91324E-01   5.56E-09
Np02CO3-                           Np02CO3-  1.33729E-07   2.43181E-07   1.818     4.65756E-08   1.19725E-07   3.93964E-02   1.41E-12
CO2(aq)                            CO2(aq)   8.51877E-08   2.47357E-07   2.904     2.96694E-08   7.62669E-08   3.35649E-03   -1.94E-08
Np02+                              Np02+     6.18630E-09   1.22804E-08   1.985     2.15458E-09   5.53847E-09   1.49011E-03   -2.69E-09
Np02OH(aq)                         Np02OH(aq)  1.65046E-10  1.65046E-10  1.000     5.74825E-11   1.47762E-10   4.22680E-05   8.12E-09
H+                                 H+        5.76161E-11   2.25258E-10   3.910     2.00667E-11   5.15826E-11   5.19901E-08   -1.08E-08
Np02(OH)2-                         Np02(OH)2-  9.27855E-13  2.77117E-13  0.2987    3.23156E-13   8.30690E-13   2.51750E-07   1.89E-08
HCl(aq).....to.titrate.acid.only   0.00000E+00  0.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
NaOH(aq).....to.titrate.base.only  0.00000E+00  0.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
Np02OH(aged)_____Np02OH(aged)      0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.05E+00
Np02OH(amor)_____Np02OH(amor)      0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.65E+00
Na3Np02(CO3)2(s)_DISABLED_DISABLED 0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+02
NaCl_____Halite                    0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
NaHCO3_____Nahcolite               0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.28E+00
Na2CO3.10H2O_____Natron            0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.92E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate 0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
Na2CO3.H2O_____Thermonatrite       0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.24E+00
Na3H(CO3)2.2H2O_____Trona          0.00000E+00  1.00000E+00  1.000     0.00000E+00   0.00000E+00   0.00000E+00   -4.51E+00

pH (-log[aH+]); pmH(-log[mH+])     9.6473    10.2395
Osmotic Coefficient=    1.241173
Equilibrium RH (%) =   77.816979
Ionic Strength (m) =    5.611104
Density, kg/m3     =    1188.80
fCO2(g); log[fCO2(g)]=                                7.501E-06    -5.12

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.63044423E+03
Flashing Titration #          10
# inversions for batch pbln          29
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.6molal NaCl  FMT V2.1
DATABASE:  HDN84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRER89,FRP90,P91,RFFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 (=) ATM      Temperature=     2.98E+02 (=) Kelvin

Elemental Abundances for Flash Problem

  Total Moles     Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.86758077E+01  1.11018508E+02   9.93928423E+01   1.00178046E+05  Hydrogen
  3.67206779E+01  5.55237521E+01   4.97085056E+01   7.95306265E+05  Oxygen
  5.42998773E+00  5.61001154E+00   5.02254085E+00   1.15467059E+05  Sodium
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95147452E+00  5.60168756E+00   5.01508853E+00   1.77799934E+05  Chlorine
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47723877E+00  4.66287109E-03   4.17458330E-03   5.01409200E+01  Carbon
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00  4.08213591E-06   3.65466170E-06   8.66330978E-01  Np(V)
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00  0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.76219826E-15 -5.05837199E-15  -4.52866803E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     462.587531269118      grams
    H2O MASS          348.372611719453      grams
    TDS(g/kg)         327.852752218200      g/kgH2O

  Specified Solution Density
    DENSITY           1188.80231065170      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL      0.389120652882589     liters
    TDS               293.520579551782      g/l

  Density based on TDS and NaCl solutions    1188.80231065170      g/l
  Percent relative error vs NaCl density     0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                       Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                WATER     8.31901E-01   7.78190E-01   0.9354    1.93377E+01   4.96959E+01   8.95282E+05
Na3Np02CO3(s)_____Na3Np02CO3(s)   9.97672E+00   1.00000E+00   1.000     3.47561E+00   8.93197E+00   3.14446E+06
Na+                                Na+       5.61001E+00   5.28779E+00   0.9426    1.95417E+00   5.02254E+00   1.15467E+05
Cl-                                Cl-       5.60169E+00   5.27933E+00   0.9425    1.95147E+00   5.01509E+00   1.77800E+05
CO3=                               CO3=      3.58175E-03   9.29893E-05   2.5962E-02  1.24778E-03   3.20667E-03   1.92430E+02
HCO3-                              HCO3-     1.07138E-03   3.96412E-04   0.3700    3.73239E-04   9.59185E-04   5.85267E+01
OH-                                OH-       7.38545E-05   4.01754E-05   0.5440    2.57289E-05   6.61206E-05   1.12453E+00   -2.83E-10
Np02(CO3)2=-                       Np02(CO3)2=-  2.28868E-06  5.94773E-11  2.5988E-05  7.97312E-07  2.04901E-06  7.97199E-01   1.88E-09
Np02(CO3)3=5-                      Np02(CO3)3=5- 1.65423E-06  1.32488E-15  8.0090E-10  5.76289E-07  1.48100E-06  6.65081E-01   3.89E-09
Np02CO3-                           Np02CO3-  1.33749E-07   2.43195E-07   1.818     4.65965E-08   1.19743E-07   3.94022E-02   1.07E-12
CO2(aq)                            CO2(aq)   7.44762E-08   2.16257E-07   2.904     2.59455E-08   6.66772E-08   2.93445E-03   -1.54E-08
Np02+                              Np02+     5.31533E-09   1.05475E-08   1.984     1.85172E-09   4.75872E-09   1.28032E-03   -1.85E-09
Np02OH(aq)                         Np02OH(aq)  1.63595E-10  1.63595E-10  1.000     5.69919E-11   1.46463E-10   4.18964E-05   6.59E-09
H+                                 H+        4.99485E-11   1.95194E-10   3.908     1.74007E-11   4.47180E-11   4.50712E-08   -8.45E-09
Np02(OH)2-                         Np02(OH)2-  1.06147E-12  3.16997E-13  0.2986    3.69789E-13   9.50319E-13   2.88005E-07   1.50E-08
HCl(aq).....to.titrate.acid.only   0.00000E+00   0.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
NaOH(aq).....to.titrate.base.only  0.00000E+00   0.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
Np02OH(aged)_____Np02OH(aged)      0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.06E+00
Np02OH(amor)_____Np02OH(amor)      0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.65E+00
Na3Np02(CO3)2(s)_DISABLED_DISABLED 0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+02
NaCl_____Halite                    0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -1.25E-01
NaHCO3_____Nahcolite               0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.28E+00
Na2CO3.10H2O_____Natron            0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.85E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate 0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.89E+00
Na2CO3.H2O_____Thermonatrite       0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -3.18E+00
Na3H(CO3)2.2H2O_____Trona          0.00000E+00   1.00000E+00   1.000     0.00000E+00   0.00000E+00   0.00000E+00   -4.44E+00

pH (-log[aH+]); pmH(-log[mH+])     9.7095    10.3015
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
 Osmotic Coefficient=    1.241102
 Equilibrium RH (%) =   77.818980
 Ionic Strength (m) =    5.613617
 Density, kg/ml     =    1188.80
 fCO2(g); log[fCO2(g)]=                                    6.558E-06    -5.18

 NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
         - Gas "molality" and "activity" are gas partial pressures
         - "Descriptor" means:
           "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
           "Saturation Index for minerals, SI=log10(IAP/Ksp)
           "log10(activity) for aqueous species with very small concentrations
           "log10(partial pressure) for gases

 Total G/RT=    -4.63902442E+03
 Flashing Titration #          11
 # inversions for batch pblm          29
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  PMT V2.3
 DATABASE:  HDM84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

 Elemental Abundances for Flash Problem

   Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.86856177E+01  1.11018527E+02  9.93930232E+01  1.0017822E+05  Hydrogen
  3.67262240E+01  5.55243148E+01  4.97099866E+01  7.95329959E+05  Oxygen
  5.43049456E+00  5.61001334E+00  5.02255073E+00  1.15467286E+05  Sodium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
  1.95161969E+00  5.60065567E+00  5.01417296E+00  1.77767474E+05  Chlorine
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
  3.47741911E+00  5.17999317E-03  4.63756089E-03  5.57617439E+01  Carbon
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Neglon
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Th(IV)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
  3.47561578E+00  4.89951736E-06  4.38645561E-06  1.03980141E+00  Np(V)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  ClO4-(EL)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electron
 -1.67462183E-15 -4.80574176E-15 -4.30249989E-15  0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      462.705395278232      grams
    H2O MASS           348.462717099515      grams
    TDS(g/kg)          327.867636411822      g/kgH2O

  Specified Solution Density
    DENSITY            1188.79968901563      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.389220656392809       liters
    TDS                293.516483008603      g/l

  Density based on TDS and NaCl solutions     1188.79968901563      g/l
  Percent relative error vs NaCl density      0.000000000000000E+000 %


 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

 Species Name                              Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

 H2O                              WATER    8.31907E-01   7.78210E-01   0.9355        1.93427E+01   4.96960E+01   8.95283E+05
 NaNpO2CO3(s)_____________NaNpO2CO3(s)    9.97413E+00   1.00000E+00   1.000         3.47561E+00   8.92968E+00   3.14366E+06
 Na+                              Na+      5.61001E+00   5.28749E+00   0.9425        1.95488E+00   5.02255E+00   1.15467E+05
 Cl-                              Cl-      5.60066E+00   5.27780E+00   0.9424        1.95162E+00   5.01417E+00   1.77767E+05
 CO3=                             CO3=     4.08730E-03   1.06108E-04   2.5960E-02    1.42427E-03   3.65929E-03   2.19591E+02
 HCO3-                            HCO3-    1.08082E-03   3.99866E-04   0.3700        3.76626E-04   9.67642E-04   5.90427E+01
 OH-                              OH-      8.35413E-05   4.54485E-05   0.5440        2.91110E-05   7.47929E-05   1.27203E+00   -2.22E-10
 NpO2(CO3)2=-                     NpO2(CO3)2=-  2.61033E-06  6.78722E-11  2.6001E-05  9.09603E-07  2.33699E-06  9.09240E-01   1.36E-09
 NpO2(CO3)3=5-                    NpO2(CO3)3=5-  2.15059E-06  1.72518E-15  8.0219E-10  7.49402E-07  1.92539E-06  8.64644E-01   2.85E-09
 NpO2CO3-                         NpO2CO3-  1.33768E-07   2.43209E-07   1.818         4.66133E-08   1.19761E-07   3.94080E-02   8.21E-13
 CO2(aq)                          CO2(aq)   6.64082E-08   1.92831E-07   2.904         2.31408E-08   5.94541E-08   2.61656E-03   -1.26E-08
 NpO2+                            NpO2+     4.66017E-09   9.24400E-09   1.984         1.62390E-09   4.17217E-09   1.12251E-03   -1.34E-09
 NpO2OH(aq)                       NpO2OH(aq)  1.62195E-10  1.62195E-10  1.000         5.65189E-11   1.45210E-10   4.15381E-05   5.50E-09
 H+                               H+        4.41741E-11   1.72551E-10   3.906         1.53930E-11   3.95483E-11   3.98608E-08   -6.85E-09
 NpO2(OH)2-                       NpO2(OH)2-  1.19063E-12  3.55535E-13  0.2986        4.14889E-13   1.06595E-12   3.23048E-07   1.24E-08
 HCl(aq).....to.titrate.acid.only          0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
 NaOH(aq).....to.titrate.base.only         0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
 NpO2OH(aged)_____________NpO2OH(aged)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.06E+00
 NpO2OH(amor)_____________NpO2OH(amor)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.66E+00
 Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+02
 NaCl_____________________________Halite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.25E-01
 NaHCO3___________________________Nahcolite  0.00000E+00  1.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.27E+00
 Na2CO3.10H2O_____________________Natron   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.79E+00
 Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.83E+00
 Na2CO3.H2O_____________Thermonatrite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.12E+00
 Na3H(CO3)2.2H2O_____________Trona         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.36E+00

 pH (-log[aH+]); pmH(-log[mH+])       9.7631       10.3548
 Osmotic Coefficient=    1.241031
 Equilibrium RH (%) =   77.820979
 Ionic Strength (m) =    5.614130
 Density, kg/ml     =    1188.80
 fCO2(g); log[fCO2(g)]=                                    5.848E-06    -5.23

 NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
         - Gas "molality" and "activity" are gas partial pressures
         - "Descriptor" means:
           "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
           "Saturation Index for minerals, SI=log10(IAP/Ksp)
           "log10(activity) for aqueous species with very small concentrations
           "log10(partial pressure) for gases

 Total G/RT=    -4.63960458E+03
 Flashing Titration #          12
 # inversions for batch pblm          29
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  PMT V2.3
 DATABASE:  HDM84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

 Elemental Abundances for Flash Problem

   Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
  3.86958278E+01   1.11018546E+02   9.93932031E-01   1.00178409E+05  Hydrogen
  3.67317700E+01   5.55258769E+01   4.97114666E-01   7.95353639E+05  Oxygen
  5.43100040E+00   5.61001519E+00   5.02256062E-02   1.15467513E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95176486E+00   5.59962430E+00   5.01325782E+00   1.77735029E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47759944E+00   5.69691170E-03   5.10035774E-03   6.12603968E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   5.78031156E-06   5.17502615E-06   1.22673061E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.60809713E-15  -4.61363967E-15  -4.13052089E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS      462.823267120614      grams
   H2O MASS           348.552823457537      grams
   TDS(g/kg)          327.842541998512      g/kgH2O

 Specified Solution Density
   DENSITY            1188.79707833404      kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL     0.389320663345848       liters
   TDS              293.512403582768        g/l

 Density based on TDS and NaCl solutions     1188.79707833404      g/l
 Percent relative error vs NaCl density      0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                  WATER  8.31913E-01   7.78230E-01   0.9355        1.93477E+01   4.96961E+01   8.95285E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.97156E+00   1.00000E+00    1.000        3.47561E+00   8.92738E+00   3.14285E+06
Na+                                  Na+    5.61002E+00   5.28718E+00   0.9425        1.95539E+00   5.02256E+00   1.15466E+05
Cl-                                  Cl-    5.59962E+00   5.27626E+00   0.9423        1.95176E+00   5.01326E+00   1.77735E+05
CO3+                                 CO3+   4.59262E-03   1.19219E-04   2.5959E-02    1.60077E-03   4.11170E-03   2.46740E+02
HCO3-                                HCO3-  1.09010E-03   4.03260E-04   0.1699        3.79959E-04   9.75854E-04   5.95499E+01
OH-                                  OH-    9.30687E-05   5.06360E-05   0.5441        3.24393E-05   8.33210E-05   1.41710E+00  -1.82E-10
Np02(CO3)2+-                  Np02(CO3)2+-  2.93150E-06   7.62632E-11   2.6015E-05    1.02178E-06   2.62452E-06   1.02111E+00   1.03E-09
Np02(CO3)3++-                 Np02(CO3)3++- 2.71072E-06   2.17799E-15   8.0347E-10    9.44829E-07   2.42687E-06   1.08984E+00   2.18E-09
Np02CO3-                        Np02CO3-    1.33788E-07   2.43223E-07    1.818        4.66322E-08   1.19778E-07   3.94138E-02   6.48E-13
CO2(aq)                            CO2(aq)  6.01101E-08   1.74545E-07    2.904        2.09515E-08   5.38156E-08   2.36842E-03  -1.06E-08
Np02+                              Np02+    4.14945E-09   8.22786E-09    1.983        1.44630E-09   3.71494E-09   9.99493E-04  -1.01E-09
Np02OH(aq)                    Np02OH(aq)    1.60844E-10   1.60844E-10    1.000        5.60625E-11   1.44001E-10   4.11921E-05   4.70E-09
H+                                   H+     3.96673E-11   1.54678E-10    3.904        1.38262E-11   3.55135E-11   3.57941E-08  -5.71E-09
Np02(OH)2-                    Np02(OH)2-    1.31559E-12   3.92815E-13   0.2986        4.58552E-13   1.17783E-12   3.56954E-07   1.04E-08
HCl(aq).....to.titrate.acid.only           0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -2.49E+02
NaOH(aq).....to.titrate.base.only          0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -2.94E+02
Np02OH(aged)_____________Np02OH(aged)      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -3.07E+00
Np02OH(amor)_____________Np02OH(amor)      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -3.66E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -9.31E+02
NaCl_____________________________Halite    0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -1.25E-01
NaHCO3___________________________Nahcolite 0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -2.27E+00
Na2CO3.10H2O_____________________Natron    0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -2.74E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -2.78E+00
Na2CO3.H2O_____________Thermonatrite       0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -1.97E+00
Na3H(CO3)2.2H2O_________________Trona      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00  -4.32E+00

pH (-log[aH+]); pmH(-log[mH+])       8.8100      10.4016
Osmotic Coefficient=     1.240960
Equilibrium RH (%) =    77.822977
Ionic Strength (m) =     5.614644
Density, kg/m3     =     1188.80
fCO2(g); log[fCO2(g)]=                                    5.293E-06    -5.28

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals. SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=     -4.64018472E+03
Flashing Titration #          13
# inversions for batch pblm          29
1Benchmark TITRATE Problem, LINEAR option: Np(V)O2 with CO3 in 5.6molal NaCl  FMT V2.3
 DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NRB94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR85,FRF90,P91,RFVR92,RFF96,RRFF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

 Elemental Abundances for Flash Problem

   Total Moles=      Aq. Molality      Aq. Molarity      Aq. mg/liter
  3.87058378E+01   1.11018565E+02   9.93933820E+01   1.00178590E+05  Hydrogen
  3.67373160E+01   5.55274383E+01   4.97129457E+01   7.95377304E+05  Oxygen
  5.43150623E+00   5.61001708E+00   5.02257052E+00   1.15467741E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95191003E+00   5.59859345E+00   5.01234310E+00   1.77702600E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47777977E+00   6.21362642E-03   5.56297360E-03   6.68168759E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   6.72405267E-06   6.01995114E-06   1.42701858E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.01294383E-15  -2.90539042E-15  -2.60115577E-15   0.00000000E+00  Charge
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
1727   Solution Parameters, Calculated
1728     SOLUTION MASS      462.941146744387      grams
1729     H2O MASS           348.642930744907      grams
1730     TDS(g/kg)          327.837468998068
1731
1732   Specified Solution Density
1733     DENSITY            1188.79447861716      kg/m^3 = g/l
1734
1735   Solution Parameters Based on Specified Density
1736     SOLUTION VOL     0.389420673691967       liters
1737     TDS               293.508341290296       g/l
1738
1739   Density based on TDS and NaCl solutions     1188.79447861716      g/l
1740   Percent relative error vs NaCl density    0.000000000000000E+000 %
1741
1742
1743
1744   TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1745
1746   Species Name                          Molality     Activity     Act Coef     Total Moles   Molarity     mg/liter     Descriptor
1747
1748   H2O                          WATER    8.31920E-01  7.78250E-01  0.9355       1.93527E+01  6.96962E+01  8.95286E+05
1749   NaNpO2CO3(s)_____NaNpO2CO3(s)         9.96898E+00  1.00000E+00   1.000       3.47561E+00  8.92509E+00  3.14204E+06
1750   Na+                           Na+     5.61002E+00  5.28688E+00  0.9424       1.95589E+00  5.02257E+00  1.15468E+05
1751   Cl-                           Cl-     5.59859E+00  5.27473E+00  0.9422       1.95191E+00  5.01234E+00  1.77703E+05
1752   CO3=                          CO3=    5.09770E-03  1.32323E-04  2.5957E-02   1.77728E-03  4.56390E-03  2.73676E+02
1753   HCO3-                         HCO3-   1.09923E-03  4.06595E-04  0.3699       3.83240E-04  9.84128E-04  6.00486E+01
1754   OH-                           OH-     1.02445E-04  5.57417E-05  0.5441       3.57166E-05  9.17172E-05  1.55986E+00  -1.54E-10
1755   NpO2(CO3)3---          NpO2(CO3)3---  3.33418E-06  2.68321E-15  8.0476E-10   1.16244E-06  2.98505E-06  1.34051E+00   1.71E-09
1756   NpO2(CO3)2--           NpO2(CO3)2--   3.25216E-06  8.46501E-11  2.6029E-05   1.13384E-06  2.91162E-06  1.13281E+00   7.96E-10
1757   NpO2CO1-                    NpO2CO3-  1.33807E-07  2.43217E-07   1.818       4.66510E-08  1.19796E-07  3.94186E-02   5.37E-13
1758   CO2(aq)                       CO2(aq) 5.50552E-08  1.59869E-07  2.904        1.91946E-08  4.92902E-08  2.16925E-03  -9.11E-09
1759   NpO2+                         NpO2+   3.74015E-09  7.41351E-09  1.982        1.30398E-09  3.34851E-09  9.00905E-04  -7.82E-10
1760   NpO2OH(aq)                 NpO2OH(aq) 1.59537E-10  1.59537E-10  1.000        5.56216E-11  1.42832E-10  4.08578E-05   4.10E-09
1761   H+                            H+      1.60509E-11  1.40695E-10  3.903        1.25689E-11  3.22759E-11  3.25308E-08  -4.88E-09
1762   NpO2(OH)2-                 NpO2(OH)2- 1.43661E-12  4.28912E-13  0.2986       5.00864E-13  1.28618E-12  1.89791E-07   8.98E-09
1763   HCl(aq).....to.titrate.acid.only      0.00000E+00  0.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.49E+02
1764   NaOH(aq).....to.titrate.base.only     0.00000E+00  0.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.94E+02
1765   NpO2OH(aged)_____________NpO2OH(aged) 0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.07E+00
1766   NpO2OH(amor)_____________NpO2OH(amor) 0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.66E+00
1767   Na3NpO2(CO3)2(s)_DISABLED_DISABLED    0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -9.31E+02
1768   NaCl_____________________Halite       0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.25E-01
1769   NaHCO3___________________Nahcolite    0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.26E+00
1770   Na2CO3.10H2O_____________Natron       0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.70E+00
1771   Na2CO3.7H2O____Na2CO3-Heptahydrate    0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.73E+00
1772   Na2CO3.H2O_____________Thermonatrite  0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.02E+00
1773   Na3H(CO3)2.2H2O_____________Trona     0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -4.27E+00
1774
1775   pH (-log[aH+]); pmH(-log[mH+])      9.8517       10.4431
1776   Osmotic Coefficient=    1.240888
1777   Equilibrium RH (%) =   77.824974
1778   Ionic Strength (m) =    5.615158
1779   Density, kg/m3     =    1188.79
1780   fCO2(g); log[fCO2(g)]=                                4.848E-06    -5.31
1781
1782   NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
1783           - Gas "molality" and "activity" are gas partial pressures
1784           - "Descriptor" means:
1785             *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
1786             *Saturation Index for minerals, SI=log10(IAP/Ksp)
1787             *log10(activity) for aqueous species with very small concentrations
1788             *log10(partial pressure) for gases
1789
1790   Total G/RT=     -4.64076481E+03
1791   Flashing Titration #          14
1792   # inversions for batch pblm          29
1793 1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
1794   DATABASE:  NMM84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1795   95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,991,RFFR92,RFF94,RRFF94)
1796      Pressure=     1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin
1797
1798   Elemental Abundances for Flash Problem
1799
1800     Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter
1801
1802     3.87158478E+01    1.11018583E+02    9.93935600E+01    1.00178769E+05  Hydrogen
1803     3.67428620E+01    5.55289991E+01    4.97144239E+01    7.95400954E+05  Oxygen
1804     5.43201206E+00    5.61001902E+00    5.02258043E+00    1.15467969E+05  Sodium
1805     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
1806     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
1807     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
1808     1.95205520E+00    5.59756111E+00    5.01142881E+00    1.77670186E+05  Chlorine
1809     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
1810     3.47796010E+00    6.73011708E-03    6.02540822E-03    7.23711783E+01  Carbon
1811     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  PosIon
1812     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  NegIon
1813     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
1814     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
1815     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
1816     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
1817     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Tb(IV)
1818     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
1819     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
1820     3.47561578E+00    7.73027765E-06    6.92082168E-06    1.64056832E+00  Np(V)
1821     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
1822     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
1823     0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
1824    -1.48913390E-15   -4.27012565E-15   -3.82299052E-15    0.00000000E+00  Charge
1825
1826   Solution Parameters, Calculated
1827     SOLUTION MASS      463.059034099430      grams
1828     H2O MASS           348.731038917603      grams
1829     TDS(g/kg)          327.832417417837      g/kgH2O
1830
1831   Specified Solution Density
1832     DENSITY            1188.79188986888      kg/m^3 = g/l
1833
1834   Solution Parameters Based on Specified Density
1835     SOLUTION VOL     0.389520687384993       liters
1836     TDS               293.504296137241       g/l
1837
1838   Density based on TDS and NaCl solutions     1188.79188986888      g/l
1839   Percent relative error vs NaCl density    0.000000000000000E+000 %
1840
1841
1842
1843   TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1844
1845   Species Name                          Molality     Activity     Act Coef     Total Moles   Molarity     mg/liter     Descriptor
1846
1847   H2O                          WATER    8.31926E-01  7.78270E-01  0.9355       1.93577E+01  4.96962E+01  8.95288E+05
1848   NaNpO2CO3(s)_____NaNpO2CO3(s)         9.96640E+00  1.00000E+00   1.000       3.47561E+00  8.92279E+00  3.14123E+06
1849   Na+                           Na+     5.61002E+00  5.28658E+00  0.9423       1.95640E+00  5.02258E+00  1.15468E+05
1850   Cl-                           Cl-     5.59756E+00  5.27320E+00  0.9421       1.95206E+00  5.01143E+00  1.77670E+05
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
CO3=                          CO3=     5.60253E-03  1.45416E-04  2.5956E-02   1.95179E-03  5.01588E-03  3.00999E+02
HCO3-                         HCO3-    1.10821E-03  4.09875E-04  0.3699       3.86471E-04  9.92171E-04  6.05394E+01
OH-                           OH-      1.11676E-04  6.07695E-05  0.5442       3.89450E-05  9.99819E-05  1.70042E+00  -1.34E-10
Np02(CO3)3=4-        Np02(CO3)3=4-     4.02056E-06  3.24077E-15  8.0605E-10   1.40210E-06  3.59956E-06  1.61647E+00   1.38E-09
Np02(CO3)2=-         Np02(CO3)2=-      3.57213E-06  9.30328E-11  2.6043E-05   1.24579E-06  3.19826E-06  1.24433E+00   6.32E-10
Np02CO3-                   Np02CO3-    1.33827E-07  2.43251E-07  1.818        4.66698E-08  1.19813E-07  3.94254E-02   4.51E-13
CO2(aq)                       CO2(aq)  5.09071E-08  1.47825E-07  2.904        1.77530E-08  4.55765E-08  2.00581E-03  -7.97E-09
Np02+                         Np02+    3.40480E-09  6.74629E-09  1.981        1.18737E-09  3.04837E-09  8.20129E-04  -6.21E-10
Np02OH(aq)                 Np02OH(aq)  1.58274E-10  1.58274E-10  1.000        5.51952E-11  1.41700E-10  4.05340E-05   3.62E-09
H+                                H+   3.30838E-11  1.25058E-10  3.901        1.15374E-11  2.96195E-11  2.98535E-08  -4.24E-09
Np02(OH)2-                 Np02(OH)2-  1.55392E-12  4.63895E-13  0.2985       5.41903E-13  1.39121E-12  4.21621E-07   7.87E-09
HCl(aq).....to.titrate.acid.only      0.00000E+00  0.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.49E+02
NaOH(aq).....to.titrate.base.only     0.00000E+00  0.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.94E+02
Np02OH(aged)_____________Np02OH(aged) 0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -3.07E+00
Np02OH(amor)_____________Np02OH(amor) 0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -3.67E+00
NaJNp02(CO3)2(s)_DISABLED_DISABLED    0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -9.31E+02
NaCl_____________________Halite       0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -1.25E-01
NaHCO3___________________Nahcolite    0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.26E+00
Na2CO3.10H2O_____________Natron       0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.66E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate    0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.66E+00
Na2CO3.H2O_____Thermonatrite          0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.98E+00
NaJH(CO3)2.2H2O__________Trona        0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -4.23E+00

pH (-log[aH+]); pmH(-log[mH+])        9.8892       10.4804
Osmotic Coefficient=     1.240817
Equilibrium RH (%) =    77.826970
Ionic Strength (m) =     5.615672
Density, kg/m3     =     1188.79
fCO2(g); log(fCO2(g))=                                    4.483E-06    -5.35

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=     -4.64134493E+03
Flashing Titration #          15
# inversions for batch pblm          39
Benchmark TITRATE Problem, LINEAR option: Np(V)O2 with CO3 in 5.6imolal NaCl  FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,FRF90,P91,RFFR92,RFP94,RRFP94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

  3.87258579E+01   1.11018601E+02   9.93937371E+01   1.00178948E+05  Hydrogen
  1.67484080E+01   5.55305592E+01   4.97159013E+01   7.95424591E+05  Oxygen
  5.43251790E+00   5.61002101E+00   5.02259034E+00   1.15468197E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95220036E+00   5.59653330E+00   5.01051495E+00   1.77637786E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47814044E+00   7.24644343E-03   6.48766141E-03   7.79233012E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Poslon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Neglon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  1.47561578E+00   8.79854605E-06   7.87721651E-06   1.86728474E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.76476943E-15  -5.05820963E-15  -4.52945495E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      463.176929136620      grams
    H2O MASS           348.823147935355      grams
    TDS(g/kg)          327.627387253719      g/kgH2O

  Specified Solution Density
    DENSITY            1188.78931208719      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.389630704381509        liters
    TDS             293.500268120485         g/l

  Density based on TDS and NaCl solutions     1188.78931208719      g/l
  Percent relative error vs NaCl density      0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                          Molality     Activity     Act Coef     Total Moles  Molarity     mg/liter     Descriptor

H2O                          WATER    8.31932E-01  7.78290E-01  0.9355       1.93627E+01  4.96963E+01  8.95289E+05
NaNp02CO3(s)_____________NaNp02CO3(s) 9.96382E+00  1.00000E+00  1.000        3.47561E+00  8.92050E+00  3.14043E+06
Na+                             Na+   5.61002E+00  5.28628E+00  0.9423       1.95691E+00  5.02259E+00  1.15468E+05
Cl-                             Cl-   5.59653E+00  5.27166E+00  0.9420       1.95220E+00  5.01051E+00  1.77638E+05
CO3=                           CO3=   6.10711E-03  1.58505E-04  2.5954E-02   2.13010E-03  5.46763E-03  3.28108E+02
HCO3-                         HCO3-   1.11706E-03  4.13103E-04  0.3698       3.89655E-04  1.00009E-03  6.10225E+01
OH-                           OH-     1.20768E-04  6.57227E-05  0.5442       4.21267E-05  1.08122E-04  1.83887E+00  -1.19E-10
Np02(CO3)3=4-        Np02(CO3)3=4-    4.76942E-06  3.85055E-15  8.0734E-10   1.66368E-06  4.27001E-06  1.91755E+00   1.14E-09
Np02(CO3)2=-         Np02(CO3)2=-     3.89199E-06  1.01411E-10  2.6056E-05   1.35762E-06  3.48446E-06  1.35568E+00   5.12E-10
Np02CO3-                   Np02CO3-   1.33846E-07  2.43265E-07  1.817        4.66887E-08  1.19831E-07  3.94312E-02   3.64E-13
CO2(aq)                       CO2(aq)  4.74407E-08  1.37761E-07  2.904        1.65484E-08  4.24731E-08  1.86923E-03  -7.08E-09
Np02+                         Np02+    3.12502E-09  6.16962E-09  1.981        1.09008E-09  2.79779E-09  7.52738E-04  -5.03E-10
Np02OH(aq)                 Np02OH(aq)  1.57050E-10  1.57050E-10  1.000        5.47826E-11  1.40605E-10  4.02206E-05   3.24E-09
H+                                H+   3.06048E-11  1.19335E-10  3.899        1.06757E-11  2.74002E-11  2.76166E-08  -3.75E-09
Np02(OH)2-                 Np02(OH)2-  1.66771E-12  4.97826E-13  0.2985       5.81743E-13  1.49310E-12  4.52501E-07   6.99E-09
HCl(aq).....to.titrate.acid.only      0.00000E+00  0.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.49E+02
NaOH(aq).....to.titrate.base.only     0.00000E+00  0.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.94E+02
Np02OH(aged)_____________Np02OH(aged) 0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -3.08E+00
Np02OH(amor)_____________Np02OH(amor) 0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -3.67E+00
NaJNp02(CO3)2(s)_DISABLED_DISABLED    0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -9.31E+02
NaCl_____________________Halite       0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -1.25E-01
NaHCO3___________________Nahcolite    0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.26E+00
Na2CO3.10H2O_____________Natron       0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.62E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate    0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.66E+00
Na2CO3.H2O_____Thermonatrite          0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -2.94E+00
NaJH(CO3)2.2H2O__________Trona        0.00000E+00  1.00000E+00  1.000        0.00000E+00  0.00000E+00  0.00000E+00  -4.19E+00

pH (-log[aH+]); pmH(-log[mH+])        9.9232       10.5142
Osmotic Coefficient=     1.240746
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
1975  Equilibrium RH (%) =   77.828965
1976  Ionic Strength (m) =    5.616187
1977  Density, kg/m3     =     1188.79
1978  fCO2(g), log(fCO2(g))=                                  4.178E-06    -5.38
1979
1980  NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
1981          - Gas "molality" and "activity" are gas partial pressures
1982          - "Descriptor" means:
1983            "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
1984            "Saturation Index for minerals, SI=log10(IAP/Ksp)
1985            "log10(activity) for aqueous species with very small concentrations
1986            "log10(partial pressure) for gases
1987
1988  Total G/RT=    -4.64192502E+03
1989  TITRATE  file name is U1:[SCRABB.FMT.UM]NP_NACL_BM_LIN.TITRATE;1
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

See Table 15 for explanation of this listing.

```
INPUT    file name is:U1:[SCBASB.FMT.UM]NP_NACL_BM.IN;1
INGUESS  file name is:U1:[SCBASB.FMT.UM]NP_NACL_BM.INGUESS;1
OUTPUT   file name is:U1:[SCBASB.FMT.UM]NP_NACL_BM.OUT;2
CHEMDAT  file name is U1:[SCBASB.FMT.UM]FMT_NEW_NP_AM_RTEST.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                    FMT V2.3
DATABASE:  MMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (HR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFP94,R3FP94)

Accuracy of reactions is              1.0000E-06
Minimum elemental abundance is        1.0000E-18
Number of Aqueous Species is          50

PITZER Data Base NOT Echoed in this Run

Species Order for Pitzer Parameters

Cations    13

Na+              K+               Ca++             Mg++             MgOH+            H+
MgB(OH)4+        CaB(OH)4+        Am+++            AmCO3+           Th++++           UO2++
NpO2+

Anions     20

Cl-              SO4=             HSO4-            OH-              HCO3-            CO3=
B(OH)4-          B3O3(OH)4-       B4O5(OH)4=       Br-              Am(CO3)2-        Am(CO3)3=-
ClO4-         ps NpO2(OH)2-       NpO2CO3-         NpO2(CO3)2=-     NpO2(CO3)3=--    H2PO4-
NPO4=            PO4=-

Neutral    6

CO2(aq)          CaCO3(aq)        MgCO3(aq)        B(OH)3(aq)       NpO2OH(aq)       H3PO4(aq)

using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

this is a TITRATION problem

Ideal Gas Constant is Unity (Dimensionless)
Temperature =       298.15 [=] degrees Kelvin

  115 Species                    23 Elements

        Element Name          Molecular Weight
        Hydrogen                     1.00790
        Oxygen                      15.99940
        Sodium                      22.98977
        Potassium                   39.09830
        Magnesium                   24.30500
        Calcium                     40.08000
        Chlorine                    35.45300
        Sulfur                      32.06000
        Carbon                      12.01100
        PosIon                       0.00000
        NegIon                       0.00000
        Air                         28.84000
        Boron                       10.81000
        Bromine                     79.90400
        TracerEl                     0.00000
        Th(IV)                     232.03810
        Am(III)                    243.00000
        U(VI)                      238.02900
        Np(V)                      237.04820
        ClO4-(EL)                   99.45060
        Phosphorus                  30.97400
        Electron                     0.00000
        Charge                       0.00000

    Species Name                          Phase      Mol.Wt.    Std Chemical Potential, u/RT
  1 H2O                            WATER  aqueous     18.015      -95.6635
  2 Na+                              Na+  aqueous     22.990     -105.6510
  3 K+                                K+  aqueous     39.098     -113.9570
  4 Ca++                            Ca++  aqueous     40.080     -223.3000
  5 Mg++                            Mg++  aqueous     24.305     -183.4680
  6 MgOH+                          MgOH+  aqueous     41.312     -251.9400
  7 H+                                H+  aqueous      1.008        0.0000
  8 Cl-                              Cl-  aqueous     35.453      -52.9550
  9 SO4=                            SO4=  aqueous     96.058     -300.3860
 10 HSO4-                          HSO4-  aqueous     97.066     -304.9420
 11 OH-                              OH-  aqueous     17.007      -63.4350
 12 HCO3-                          HCO3-  aqueous     61.017     -236.7510
 13 CO3=                           CO3=   aqueous     60.009     -212.9440
 14 CO2(aq)                     CO2(aq)   aqueous     44.010     -155.6800
 15 CaCO3(aq)                CaCO3(aq)    aqueous    100.089     -443.5000
 16 MgCO3(aq)                MgCO3(aq)    aqueous     84.314     -403.1550
 17 B(OH)3(aq)               B(OH)3(aq)   aqueous     61.832     -390.8100
 18 B(OH)4-                    B(OH)4-    aqueous     78.839     -465.2000
 19 B3O3(OH)4-              B3O3(OH)4-    aqueous    148.457     -963.7700
 20 B4O5(OH)4=              B4O5(OH)4=    aqueous    191.266    -1239.1000
 21 CaB(OH)4+                CaB(OH)4+    aqueous    118.919     -692.3000
 22 MgB(OH)4+                MgB(OH)4+    aqueous    103.144     -651.8900
 23 Br-                            Br-    aqueous     79.904     -999.9900
 24 ClO4-          perchlorate ClO4-      aqueous     99.451     -999.9900
 25 NaOH(aq).....to.titrate.base.only     aqueous     39.997      500.0000
 26 HCl(aq).....to.titrate.acid.only      aqueous     36.461      500.0000
 27 HClO4(aq).....to.titrate.acid.only    aqueous    100.459      500.0000
 28 PosIon.................POSITIVE.ION   aqueous      0.000        0.0000
 29 NegIon.................NEGATIVE.ION   aqueous      0.000        0.0000
 30 PosIon(OH)(aq).....to.titrate.base    aqueous     17.007      500.0000
 31 HNegIon(aq).........to.titrate.acid   aqueous      1.008      500.0000
 32 Tracer(aq).....conservative.tracer    aqueous      0.000        0.0000
 33 H3PO4(aq)                   H3PO4(aq) aqueous     97.995     -460.9000
 34 H2PO4-                      H2PO4-    aqueous     96.987     -455.9600
 35 HPO4=                       HPO4=     aqueous     95.980     -439.3670
 36 PO4=-                       PO4=-     aqueous     94.972     -410.9470
 37 NpO2+                       NpO2+     aqueous    269.047     -369.1270
 38 NpO2OH(aq)               NpO2OH(aq)   aqueous    286.054     -438.5180
 39 NpO2(OH)2-               NpO2(OH)2-   aqueous    303.062     -505.8290
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

115	40	NpO2CO3-	NpO2CO3-	aqueous	329.056	-594.4920	
116	41	NpO2(CO3)2=-	NpO2(CO3)2=-	aqueous	389.065	-808.4030	
117	42	NpO2(CO3)3=5-	NpO2(CO3)3=5-	aqueous	449.075	-1019.9180	
118	43	Am+++	Am+++	aqueous	243.000	-241.6940	
119	44	AmCO3+	AmCO3+	aqueous	303.009	-472.0600	
120	45	Am(CO3)2-	Am(CO3)2-	aqueous	363.018	-695.8800	
121	46	Am(CO3)3=3-	Am(CO3)3=3-	aqueous	423.028	-915.4600	
122	47	Am(OH)2+	Am(OH)2+	aqueous	277.015	-393.6470	
123	48	Am(OH)3(aq)	Am(OH)3(aq)	aqueous	294.022	-462.9500	
124	49	Th++++	Th++++	aqueous	232.038	-999.9900	
125	50	UO2++	U(VI)O2++	aqueous	270.028	-999.9900	
126	51	NpO2OH(aged)	NpO2OH(aged)	solid	286.054	-454.0100	
127	52	NpO2OH(amor)	NpO2OH(amor)	solid	286.054	-452.6420	
128	53	NaNpO2CO3(s)	NaNpO2CO3(s)	solid	352.046	-713.7070	
129	54	Na3NpO2(CO3)2(s)	_DISABLED_DISABLED	solid	458.035	999.9900	
130	55	AmOHCO3(c)	AmOHCO3(c)	solid	320.017	-569.9800	
131	56	Am(OH)3(s)	Am(OH)3(s)	solid	294.022	-492.2940	
132	57	NaAm(CO3)2.6H2O(c)		solid	494.099	-1396.4940	
133	58	AmPO4(c)	AmPO4(c)	solid	337.972	-709.7500	
134	59	CaSO4	Anhydrite	solid	136.138	-533.7300	
135	60	NaK3(SO4)2	Aphthalite/Glaserite	solid	332.400	-1057.0500	
136	61	CaCl2.6H2O	Antarcticite	solid	219.077	-893.6500	
137	62	CaCO3	Aragonite	solid	100.089	-455.1700	
138	63	K2SO4	Arcanite	solid	174.254	-532.3900	
139	64	MgCl2.6H2O	Bischofite	solid	203.302	-853.1000	
140	65	Na2Mg(SO4)2.4H2O	Bloedite	solid	334.461	-1383.6000	
141	66	Mg(OH)2	Brucite	solid	58.320	-335.4000	
142	67	Na6CO3(SO4)2	Burkeite	solid	390.063	-1449.4000	
143	68	CaCO3	Calcite	solid	100.089	-455.6000	
144	69	CaCl2.4H2O	CaCl2_Tetrahydrite	solid	183.047	-698.7000	
145	70	Ca4Cl2(OH)6.13H2O	CaOxychloride A	solid	567.467	-2658.4500	
146	71	Ca2Cl2(OH)2.H2O	CaOxychloride B	solid	203.096	-778.4100	
147	72	KMgCl3.6H2O	Carnallite	solid	277.854	-1020.3000	
148	73	MgSO4.7H2O	Epsomite	solid	246.469	-1157.8300	
149	74	CaNa2(CO3)2.5H2O	Gaylussite	solid	296.154	-1360.5000	
150	75	Na2Ca(SO4)2	Glauberite	solid	278.175	-1047.4500	
151	76	CaSO4.2H2O	Gypsum	solid	172.168	-725.5600	
152	77	NaCl	Halite	solid	58.443	-154.9900	
153	78	MgSO4.6H2O	Hexahydrite	solid	228.454	-1061.6000	
154	79	KMgClSO4.3H2O	Kainite	solid	248.960	-938.2000	
155	80	KHCO3	Kalicinite	solid	100.115	-150.0600	
156	81	MgSO4.H2O	Kieserite	solid	138.378	-579.8000	
157	82	K2Mg(SO4)2.4H2O	Leonite	solid	366.678	-1403.9700	
158	83	Na4Ca(SO4)3.2H2O	Labile_Salt	solid	456.242	-1751.4500	
159	84	MgCO3	Magnesite	solid	84.314	-414.4500	
160	85	Mg2Cl(OH)3.4H2O	MgOxychloride	solid	207.146	-1029.6000	
161	86	KHSO4	Mercallite	solid	136.164	-417.5700	
162	87	Na2SO4.10H2O	Mirabilite	solid	322.189	-1471.1500	
163	88	K8H6(SO4)7	Misanite	solid	991.237	-3039.2400	
164	89	NaHCO3	Nahcolite	solid	84.007	-143.3300	
165	90	Na2CO3.10H2O	Natron	solid	286.141	-1382.7800	
166	91	MgCO3.3H2O	Nesquehonite	solid	138.360	-695.3000	
167	92	K2Mg(SO4)2.6H2O	Picromerite/Schoen	solid	402.708	-1596.1000	
168	93	Na2Ca(CO3)2.2H2O	Pirssonite	solid	242.108	-1073.1000	
169	94	K2MgCa2(SO4)4.2H2O	Polyhalite	solid	602.922	-2282.5000	
170	95	Ca(OH)2	Portlandite	solid	74.095	-162.1200	
171	96	K2CO3.3/2H2O	Potassium_Carbonate	solid	165.229	-577.3700	
172	97	K8H4(CO3)6.3H2O	K-Sequicarbonate	solid	730.919	-2555.4000	
173	98	KNaCO3.6H2O	K-Na-Carbonate	solid	230.188	-1006.8000	
174	99	K2NaH(CO3)2.2H2O	Potassium_Trona	solid	258.243	-971.7400	
175	100	K3H(SO4)2	Sesquipotassium_Sulfate	solid	310.418	-950.8000	
176	101	Na3H(SO4)2	Sesquisodium_Sulfate	solid	262.092	-919.6000	
177	102	Na2CO3.7H2O	Na2CO3-Heptahydrate	solid	232.095	-1094.9500	
178	103	KCl	Sylvite	solid	74.551	-164.8400	
179	104	K2Ca(SO4)2.H2O	Syngenite	solid	328.407	-1164.8000	
180	105	Mg2CaCl6.12H2O	Tachyhydrite	solid	517.590	-2015.9000	
181	106	Na2SO4	Thenardite	solid	142.037	-512.3500	
182	107	Na2CO3.H2O	Thermonatrite	solid	124.004	-518.8000	
183	108	Na3H(CO3)2.2H2O	Trona	solid	226.026	-960.3800	
184	109	Na2B4O7.10H2O	Borax	solid	381.367	-2224.1600	
185	110	B(OH)3	Borix_Acid_Solid	solid	61.832	-390.8800	
186	111	KB5O8.4H2O	K-Pentaborate_(30_C)	solid	293.204	-1770.2600	
187	112	K2B4O7.4H2O	K-Tetraborate_(30_C)	solid	305.493	-1663.4700	
188	113	NaBO2.4H2O	Sodium_Metaborate	solid	137.859	-761.4200	
189	114	NaB5O8.5H2O	Sodium_Pentaborate	solid	295.111	-1854.8000	
190	115	NaBO2.NaCl.2H2O	Teepleite_(20_C)	solid	160.372	-725.7700	

Truncated Name — Formula Matrix

194	1	H2O	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
195	2	Na+	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
196	3	K+	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
197	4	Ca++	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
198	5	Mg++	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
199	6	MgOH+	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
200	7	H+	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
201	8	Cl-	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
202	9	SO4=	0	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2
203	10	HSO4-	1	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
204	11	OH-	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
205	12	HCO3-	1	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
206	13	CO3=	0	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	-2
207	14	CO2(aq)	0	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
208	15	CaCO3(aq)	0	3	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
209	16	MgCO3(aq)	0	3	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
210	17	B(OH)3(aq)	3	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
211	18	B(OH)4-	4	4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-1
212	19	B3O3(OH)4-	4	7	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	-1
213	20	B4O5(OH)4=	4	9	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	-2
214	21	CaB(OH)4+	4	4	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
215	22	MgB(OH)4+	4	4	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
216	23	Br-	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-1
217	24	ClO4- pe	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-1
218	25	NaOH(aq).....to.ti	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
219	26	HCl(aq).....to.ti	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
220	27	HClO4(aq).....to.ti	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
221	28	PosIon.....	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1
222	29	NegIon.....	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	-1
223	30	PosIon(OH)(aq).....	1	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
224	31	NNegIon(aq).....	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
225	32	Tracer(aq).....cons	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
226	33	H3PO4(aq)	3	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
227	34	H2PO4-	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1
228	35	HPO4=	1	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-2
229	36	PO4=-	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-3
230	37	NpO2+	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1
231	38	NpO2OH(aq)	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
232	39	NpO2(OH)2-	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-1
233	40	NpO2CO3-	0	5	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-1
234	41	NpO2(CO3)2=-	0	8	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-3
235	42	NpO2(CO3)3=5-	0	11	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-5
236	43	Am+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	3
237	44	AmCO3+	0	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1
238	45	Am(CO3)2-	0	6	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	-1

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
239   46 Am(CO3)3--              0  9  0  0  0  0  0  0  3  0  0  0  0  0  0  0  1  0  0  0  0  0 -3
240   47 Am(OH)2+                2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  1
241   48 Am(OH)3(aq)             3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0
242   49 Th++++                  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  4
243   50 UO2++                   0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  2
244   51 NpO2OH(aged)_______     1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
245   52 NpO2OH(amor)_______     1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
246   53 NaNpO2CO3(s)_____       0  5  1  0  0  0  0  0  0  1  0  0  0  0  0  0  0  1  0  0  0  0  0
247   54 Na3NpO2(CO3)2(s)_DI     0  8  3  0  0  0  0  0  0  2  0  0  0  0  0  0  0  1  0  0  0  0  0
248   55 AmOHCO3(c)_______       1  4  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  1  0  0  0  0  0
249   56 Am(OH)3(s)_______       3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
250   57 NaAm(CO3)2.6H2O(c)_    12 12  1  0  0  0  0  0  2  0  0  0  0  0  0  0  1  0  0  0  0  0  0
251   58 AmPO4(c)_________       0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  1  0  0
252   59 CaSO4____________       0  4  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
253   60 NaK3(SO4)2__Aphthit     0  8  1  3  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
254   61 CaCl2.6H2O_______      12  6  0  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
255   62 CaCO3____________       0  3  0  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
256   63 K2SO4____________       0  4  0  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
257   64 MgCl2.6H2O_______      12  6  0  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
258   65 NaMg(SO4)2.4H2O___      8 12  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
259   66 Mg(OH)2__________       2  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
260   67 Na6CO3(SO4)2_____       0 11  6  0  0  0  0  0  2  1  0  0  0  0  0  0  0  0  0  0  0  0  0
261   68 CaCO3____________       0  3  0  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
262   69 CaCl2.4H2O_____CaC      8  4  0  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
263   70 Ca4Cl2(OH)6.13H2O__    32 19  0  0  0  0  4  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
264   71 Ca2Cl2(OH)2.H2O____     4  3  0  0  0  0  2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
265   72 KMgCl3.6H2O_______     12  6  0  1  1  0  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
266   73 MgSO4.7H2O________     14 11  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
267   74 CaNa2(CO3)2.5H2O____   10 11  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
268   75 Na2Ca(SO4)2_____        0  8  2  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
269   76 CaSO4.2H2O_____         4  6  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
270   77 NaCl_____________       0  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
271   78 MgSO4.6H2O_______      12 10  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
272   79 KMgClSO4.3H2O_____      4  7  0  1  1  0  0  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
273   80 KHCO3____________       1  3  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
274   81 MgSO4.H2O_____          3  5  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
275   82 K2Mg(SO4)2.4H2O____     8 12  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
276   83 Na4Ca(SO4)3.2H2O____    4 14  4  0  0  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
277   84 MgCO3____________       0  3  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
278   85 Mg2Cl(OH)3.4H2O_____   11  7  0  0  2  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
279   86 KHSO4____________       1  4  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
280   87 Na2SO4.10H2O_____      20 14  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
281   88 K6H6(SO4)7_____         6 28  0  8  0  0  0  7  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
282   89 NaHCO3___________       1  3  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
283   90 Na2CO3.10H2O_____      20 13  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
284   91 MgCO3.3H2O_____         6  6  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
285   92 K2Mg(SO4)2.6H2O Pic    12 16  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
286   93 Na2Ca(CO3)2.2H2O____    4  8  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
287   94 K2MgCa2(SO4)4.2H2O_     4 18  0  2  1  2  0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
288   95 Ca(OH)2__________       2  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
289   96 K2CO3.3/2H2O____Pota    3  4  0  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
290   97 K8H4(CO3)6.3H2O___K    10 21  0  8  0  0  0  0  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0
291   98 KNaCO3.6H2O_____       12  9  1  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
292   99 K2NaH(CO3)2.2H2O____    5  8  1  2  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
293  100 K3H(SO4)2__Sesquipo     1  8  0  3  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
294  101 Na3H(SO4)2____Sesqu     1  8  3  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
295  102 Na2CO3.7H2O____Na2C    14 10  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
296  103 KCl_____________       0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
297  104 K2Ca(SO4)2.H2O_____    2  5  0  2  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
298  105 Mg2CaCl6.12H2O_____   24 12  0  0  2  1  6  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
299  106 Na2SO4__________       0  4  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
300  107 Na2CO3.H2O_____        2  4  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
301  108 Na3H(CO3)2.2H2O____    5  8  3  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0
302  109 Na2B4O7.10H2O_____    20 17  2  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0  0
303  110 B(OH)3_____________B   3  3  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
304  111 KB5O8.4H2O____K-Pen    8 12  0  1  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0  0
305  112 K2B4O7.4H2O___K-Tet    8 11  0  2  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0  0
306  113 NaBO2.4H2O_____So      8  6  1  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
307  114 NaB5O8.5H2O_____Sod   10 13  1  0  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0  0
306  115 NaBO2.NaCl.2H2O___T    4  4  2  0  0  0  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
```

****

```
RHOMIN    file name is U1:[SCHARR.FMT.UM]FMT_HMM_NP_AM_RTEST.RHOMIN;1
# inversions for batch pblm          56
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                    FMT V2.3
DATABASE:  HDM84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,PRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

  1.11017363E+02  1.11029658E+02  1.00100314E+02  1.00891107E+05  Hydrogen
  6.15086815E+01  6.15154934E+01  5.54601388E+01  8.87328944E+05  Oxygen
  5.61000000E+00  5.61062129E+00  5.05813276E+00  1.16289807E+05  Sodium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
  1.61000000E+00  1.61017838E+00  1.45167838E+00  5.14663538E+04  Chlorine
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
  2.00000001E+00  2.00022150E+00  1.80332719E+00  2.16597629E+04  Carbon
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  PosIon
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  NegIon
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Th(IV)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Np(V)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  ClO4-(EL)
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electren
 -1.77635684E-15 -1.77655156E-15 -1.60167629E-15  0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      1306.07033909890       grams
    H2O MASS           999.889265717486       grams
    TDS(g/kg)          306.214981877726       g/kgH2O

  Specified Solution Density
    DENSITY            1177.63607439302       kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL       1.10906108219560       liters
    TDS                276.072326670473       g/l

  Density Based on TDS and NaCl solutions     1177.63607439302      g/l
  Percent relative error vs NaCl density   0.000000000000000E+000 %
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                  WATER    8.57464E-01   8.59843E-01    1.003        5.55025E+01   5.00446E+01   9.01564E+05
Na+                                   Na+     5.61062E+00   3.69881E+00    0.6593       5.61000E+00   5.05833E+00   1.16290E+05
CO3=                                  CO3=    1.99407E+00   4.09214E-02    2.0522E-02   1.99385E+00   1.79778E+00   1.07884E+05
Cl-                                   Cl-     1.61018E+00   1.06477E+00    0.6613       1.61000E+00   1.45168E+00   5.14664E+04
HCO3-                                 HCO3-   6.14734E-03   1.59044E-03    0.2587       6.14666E-03   5.54222E-03   3.38170E+02
OH-                                   OH-     6.14733E-03   4.86901E-03    0.7921       6.14665E-03   5.54221E-03   9.42560E+01    2.07E-11
CO2(aq)                              CO2(aq)  2.36876E-09   7.15913E-09    3.022        2.36850E-09   2.13559E-09   9.39866E-05   -2.10E-07
H+                                    H+      2.39954E-12   1.77959E-12    0.7416       2.39927E-12   2.16334E-12   2.18043E-09   -8.49E-08
HCl(aq).....to.titrate.acid.only      HCl     0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+02
NaOH(aq).....to.titrate.base.only     NaOH    0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.92E+02
Na2CO3.10H2O_____Natron               Na2CO3  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -8.30E-02
Na2CO3.H2O_____Thermonatrite          Na2CO3  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.99E-01
Na2CO3.7H2O____Na2CO3-Heptahydrate    Na2CO3  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.51E-01
NaHCO3_____Nahcolite                  NaHCO3  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.83E+00
NaCl_____Halite                       NaCl    0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -9.75E-01
Na3H(CO3)2.2H2O_____Trona             Na3H(CO3)2.2H2O  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.57E+00

pH (-log[aH+]); pmH(-log[mH+])     11.7497      11.6199
Osmotic Coefficient=     0.908416
Equilibrium RH (%) =    85.984284
Ionic Strength (m) =     7.604695
Density, kg/m3     =     1177.64
fCO2(g); log[fCO2(g)]=                                    2.171E-07    -6.66

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -6.42133776E+03

Reaction #            1 eldsum    2.00000000000000
This is a solid-only reaction

shifting left by     4.64434654478256
calling makenuv for allomorphic reactions
# inversions for batch pbln          99
1Benchmark TITRATE Problem: Np(V)O2 with CO3 in 5.61molal NaCl                    FMT V2.3
DATABASE:  HMW84/PWB6; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  1.11018363E+02   1.11017591E+02   9.93038868E+01   1.00169020E+05  Hydrogen
  1.05508682E+02   5.55113597E+01   4.96942389E+01   7.95078006E+05  Oxygen
  1.56100000E+01   5.61057382E+00   5.02263116E+00   1.15469181E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  5.61100000E+00   5.61096098E+00   5.02297975E+00   1.78079701E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  1.00000000E+01   6.12839260E-04   5.48618892E-04   6.58946151E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Fe2ion
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Mg2ion
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  1.00000000E+01   6.12839260E-04   5.48618892E-04   1.30049121E+02  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
-4.28740972E-15  -4.28737990E-15  -3.83809877E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      1328.11614865108      grams
    H2O MASS           1000.00695466820      grams
    TDS(g/kg)          328.106912108174      g/kgH2O

  Specified Solution Density
    DENSITY            1188.93254605458      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     1.11706602116190        liters
    TDS              293.7240841133903       g/l

  Density based on TDS and NaCl solutions     1188.93254605458      g/l
  Percent relative error vs NaCl density    0.0000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                  WATER    8.31822E-01   7.77959E-01    0.9352       5.55091E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)         NaNpO2CO3(s)  9.99932E+00   1.00000E+00    1.000        9.99939E+00   8.95147E+00   3.15133E+06
Cl-                                   Cl-     5.61096E+00   5.29329E+00    0.9434       5.61100E+00   5.02298E+00   1.78080E+05
Na+                                   Na+     5.61057E+00   5.29268E+00    0.9433       5.61061E+00   5.02263E+00   1.15469E+05
NpO2+                                 NpO2+   6.12705E-04   1.21978E-03    1.991        6.12709E-04   5.48499E-04   1.47572E+02
CO2(aq)                              CO2(aq)  3.86103E-04   1.12115E-03    2.904        3.86106E-04   3.45643E-04   1.52117E+01
HCO3-                                 HCO3-   2.26571E-04   8.38810E-05    0.3702       2.26573E-04   2.02829E-04   1.23760E+01    1.23E-14
H+                                    H+      1.21872E-06   4.78095E-06    3.923        1.21873E-06   1.09101E-06   1.09962E-03    1.23E-14
NpO2CO3-                             NpO2CO3- 1.33526E-07   2.42971E-07    1.820        1.33527E-07   1.19534E-07   3.93334E-02    1.85E-14
CO3=                                  CO3=    3.09364E-08   8.03343E-10    2.5966E-02   3.09386E-08   2.76963E-08   1.66203E-03    0.00E+00
OH-                                   OH-     3.01685E-09   1.63977E-09    0.5435       3.01687E-09   2.70071E-09   4.59318E-05    1.23E-14
NpO2OH(aq)                           NpO2OH(aq) 7.72186E-10   7.72186E-10    1.000        7.72191E-10   6.91267E-10   1.97740E-04   -6.17E-15
NpO2(CO3)2=-                         NpO2(CO3)2=- 1.98304E-11   5.13355E-16    2.5877E-05   1.98385E-11   1.77595E-11   6.90960E-06    0.00E+00
NpO2(OH)2-                           NpO2(OH)2-  2.04381E-16   6.10703E-17    0.2988       2.04383E-16   1.82964E-16   5.54494E-11    0.00E+00
NpO2(CO3)3=5-                        NpO2(CO3)3=5- 1.25197E-16  9.87897E-26    7.8908E-10   1.25198E-16   1.12077E-16   5.03310E-11   -2.25E-09
HCl(aq).....to.titrate.acid.only      HCl     0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
NaOH(aq).....to.titrate.base.only     NaOH    0.00000E+00   0.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.99E+02
NpO2OH(amor)_____NpO2OH(amor)         NpO2OH(amor)  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
Na3H(CO3)2.2H2O_____Trona             Na3H(CO3)2.2H2O  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
Na2CO3.H2O_____Thermonatrite          Na2CO3  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate    Na2CO3  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.10H2O_____Natron               Na2CO3  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
NaHCO3_____Nahcolite                  NaHCO3  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
NaCl_____Halite                       NaCl    0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED    Na3NpO2(CO3)2(s)  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NpO2OH(aged)_____NpO2OH(aged)         NpO2OH(aged)  0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
pH (-log[aH+]); pmH(-log[mH+])      5.3205       5.9141
Osmotic Coefficient=    1.241871
Equilibrium RH (%) =   77.795863
Ionic Strength (m) =    5.611188
Density, kg/m3     =    1188.93
fCO2(g); log[fCO2(g)]=                                    3.400E-02    -1.47

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -1.33323084E+04
Flashing Titration #          1
# inversions for batch pblm          17
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.6lmolal NaCl                FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFP94)
    Pressure=     1.00000E+00 [=] ATM      Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

 Total Moles       Aq. Molality     Aq. Molarity     Aq. mg/liter

 3.85857174E+01  1.11017591E+02  9.93838868E+01  1.00169020E+05  Hydrogen
 3.66707638E+01  5.55113597E+01  4.96942389E+01  7.95078006E+05  Oxygen
 5.42543623E+00  5.61057382E+00  5.02263316E+00  1.15469181E+05  Sodium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
 1.95016801E+00  5.61096098E+00  5.02297975E+00  1.78079701E+05  Chlorine
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
 3.47561578E+00  6.12839260E-04  5.48618892E-04  6.58946151E+00  Carbon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  PosIon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  NegIon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Tb(IV)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
 3.47561578E+00  6.12839260E-04  5.48618892E-04  1.30049121E+02  Np(V)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  ClO4-(EL)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electron
-1.94659251E-15 -5.60067366E-15 -5.01377045E-15  0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS     461.602144251003      grams
   H2O MASS          347.563995068949      grams
   TDS(g/kg)         328.106912108174      g/kgH2O

 Specified Solution Density
   DENSITY           1188.93254605458      kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL    0.388249228926239       liters
   TDS               293.724084133903      g/l

 Density based on TDS and NaCl solutions    1188.93254605458      g/l
 Percent relative error vs NaCl density   0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                              WATER        8.31822E-01   7.77959E-01   0.9352        1.92928E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)          NaNpO2CO3(s)            9.99932E+00   1.00000E+00   1.000         3.47540E+00   8.95147E+00   3.15133E+06
Cl-                              Cl-          5.61096E+00   5.29329E+00   0.9434        1.95017E+00   5.02298E+00   1.78080E+05
Na+                              Na+          5.61057E+00   5.29268E+00   0.9433        1.95003E+00   5.02263E+00   1.15469E+05
NpO2+                            NpO2+        6.12705E-04   1.21978E-03   1.991         2.12956E-04   5.48499E-04   1.47572E+02
CO2(aq)                          CO2(aq)      3.86103E-04   1.12115E-03   2.904         1.34196E-04   3.45643E-04   1.52117E+01
HCO3-                            HCO3-        2.26571E-04   8.38810E-05   0.3702        7.87481E-05   2.02829E-04   1.23760E+01   -5.15E-12
H+                               H+           1.21872E-06   4.78095E-06   3.923         4.23582E-07   1.09101E-06   1.09962E-03   -2.29E-11
NpO2CO3-                         NpO2CO3-     1.33526E-07   2.42971E-07   1.820         4.64090E-08   1.19534E-07   3.93334E-02   1.85E-14
CO3=                             CO3=         3.09384E-08   8.03343E-10   2.5966E-02    1.07531E-08   2.76963E-08   1.66203E-03   1.68E-11
OH-                              OH-          3.01685E-09   1.63977E-09   0.5435        1.04855E-09   2.70071E-09   4.59318E-05   2.30E-11
NpO2OH(aq)                       NpO2OH(aq)   7.72186E-10   7.72186E-10   1.000         2.68384E-10   6.91267E-10   1.97740E-04   6.15E-12
NpO2(CO3)2e-                     NpO2(CO3)2e- 1.98384E-11   5.13355E-16   2.5877E-05    6.89511E-12   1.77595E-11   6.90960E-06   1.69E-11
NpO2(OH)2-                       NpO2(OH)2-   2.04381E-16   6.10703E-17   0.2988        7.10356E-17   1.82964E-16   5.54494E-11   2.92E-11
NpO2(CO3)3=-     NpO2(CO3)3=-                 1.25197E-16   9.87897E-26   7.8908E-10    4.35139E-17   1.12077E-16   5.03310E-11   -3.15E-10
HCl(aq).....to.titrate.acid.only              0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
NaOH(aq).....to.titrate.base.only             0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.99E+02
Na3H(CO3)2.2H2O_____Trona                     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
Na2CO3.H2O_____Thermonatrite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.10H2O_____Natron                       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
NaHCO3_____Nahcolite                          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
NaCl_____Halite                               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NpO2OH(amor)_____NpO2OH(amor)                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
NpO2OH(aged)_____NpO2OH(aged)                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00

pH (-log[aH+]); pmH(-log[mH+])      5.3205       5.9141
Osmotic Coefficient=    1.241871
Equilibrium RH (%) =   77.795863
Ionic Strength (m) =    5.611188
Density, kg/m3     =    1188.93
fCO2(g); log[fCO2(g)]=                                    3.400E-02    -1.47

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -4.63379813E+03
Flashing Titration #          2
# inversions for batch pblm          19
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.6lmolal NaCl                FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFP94)
    Pressure=     1.00000E+00 [=] ATM      Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.85957275E+01	1.11017746E+02	9.93891116E+01	1.00174286E+05	Hydrogen
3.66763098E+01	5.55107901E+01	4.96962723E+01	7.95110540E+05	Oxygen
5.42594206E+00	5.61014105E+00	5.02250276E+00	1.15466183E+05	Sodium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1.95031318E+00	5.60993114E+00	5.02231483E+00	1.78056128E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47579611E+00	6.99932337E-04	6.18566128E-04	7.42952570E+00	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
3.47561578E+00	1.72218651E-04	1.54179484E-04	3.65479691E+01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Clo4-(EL)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
-1.36269746E-15	-3.91969811E-15	-3.50912649E-15	0.00000000E+00	Charge

Solution Parameters, Calculated

SOLUTION MASS	461.665999617212	grams
H2O MASS	347.653675849709	grams
TDS(g/kg)	327.947988724245	g/kgH2O

Specified Solution Density

DENSITY	1188.85111378691	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	0.388329534508861	liters
TDS	293.596818859294	g/l

Density based on TDS and NaCl solutions 1188.85111378691 g/l
Percent relative error vs NaCl density 0.000000000000000E+000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31845E-01	7.78011E-01	0.9353	1.92978E+01	4.96944E+01	8.95254E+05	
NaNpO2CO3(s)	NaNpO2CO3(s)	9.99718E+00	1.00000E+00	1.000	3.47556E+00	8.95002E+00	2.15082E+06	
Na+	Na+	5.61014E+00	5.29140E+00	0.9432	1.95039E+00	5.02250E+00	1.15466E+05	
Cl-	Cl-	5.60993E+00	5.29139E+00	0.9432	1.95031E+00	5.02231E+00	1.78056E+05	
HCO3-	HCO3-	3.82212E-04	1.41513E-04	0.3702	1.32878E-04	3.42177E-04	2.08787E+01	
CO2(aq)	CO2(aq)	3.08476E-04	8.95671E-04	2.904	1.07243E-04	2.76165E-04	1.21539E+01	
NpO2+	NpO2+	1.72085E-04	3.42481E-04	1.990	5.98256E-05	1.54059E-04	4.14492E+01	-1.82E-10
H+	H+	5.77346E-07	2.26410E-06	3.922	2.00716E-07	5.16872E-07	5.20955E-04	-2.18E-10
NpO2CO3-	NpO2CO3-	1.33573E-07	2.43030E-07	1.819	4.64370E-08	1.19581E-07	3.93490E-02	8.02E-14
CO3=	CO3=	1.10196E-07	2.86188E-09	2.5971E-02	3.83099E-08	9.86531E-08	5.92010E-03	3.31E-10
OH-	OH-	6.37029E-09	3.46282E-09	0.5436	2.21466E-09	5.70303E-09	9.69932E-05	2.19E-10
NpO2OH(aq)	NpO2OH(aq)	4.57851E-10	4.57851E-10	1.000	1.59174E-10	4.09893E-10	1.17252E-04	-1.14E-10
NpO2(CO3)2=-	NpO2(CO3)2=-	7.06677E-11	1.82925E-15	2.5885E-05	2.45679E-11	6.32656E-11	2.46144E-05	3.32E-10
NpO2(CO3)3=--	NpO2(CO3)3=--	1.58546E-15	1.25406E-24	7.9097E-10	5.51192E-16	1.41939E-15	6.37412E-10	5.26E-10
NpO2(OH)2-	NpO2(OH)2-	2.55903E-16	7.64679E-17	0.2988	8.89657E-17	2.29098E-16	6.94309E-11	1.05E-10
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.45E+02
NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+02
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.61E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.21E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.36E+02
NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.72E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.36E+00
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.40E+00
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.69E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.40E+00

pH (-log[aH+]); pmH(-log[mH+]) 5.6451 6.2386
Osmotic Coefficient= 1.241740
Equilibrium RH (%) = 77.801108
Ionic Strength (m) = 5.610314
Density, kg/m3 = 1188.85
fCO2(g); log[fCO2(g)]= 2.716E-02 -1.57

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -4.63438031E+03
Flashing Titration # 1
inversions for batch pblm 28
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-Cl-Clo4 (NR94);
95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.85999827E+01	1.11017943E+02	9.93906557E+01	1.00175842E+05	Hydrogen
3.66786674E+01	5.55109442E+01	4.96970938E+01	7.95123682E+05	Oxygen
5.42615709E+00	5.61002979E+00	5.02247325E+00	1.15465482E+05	Sodium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1.95037489E+00	5.60950016E+00	5.02199809E+00	1.78044898E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47587277E+00	7.90125217E-04	7.07372710E-04	8.49625362E+00	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
3.47561578E+00	5.09865217E-05	4.56465295E-05	1.08204277E+01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Clo4-(EL)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
 -2.02795903E-15  -5.83264097E-15  -5.22176860E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS        461.701223994178        grams
    H2O MASS             347.691387425364        grams
    TDS(g/kg)            327.905265106076        g/kgH2O

  Specified Solution Density
    DENSITY              1188.82922080341        kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL      0.388366115291610          liters
    TDS                  293.562629094818        g/l

  Density based on TDS and NaCl solutions     1188.82922080341      g/l
  Percent relative error vs NaCl density    0.0000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                  WATER    8.31852E-01   7.78030E-01   0.9353        1.92999E+01   4.96951E+01   8.95267E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)        9.99622E+00   1.00000E+00   1.000         3.47560E+00   8.94928E+00   3.15056E+06
Na+                                  Na+      5.61003E+00   5.29080E+00   0.9431        1.95056E+00   5.02247E+00   1.15465E+05
Cl-                                  Cl-      5.60950E+00   5.29073E+00   0.9432        1.95037E+00   5.02200E+00   1.78045E+05
HCO3-                                HCO3-    5.79854E-04   2.14695E-04   0.3703        2.01610E-04   5.19124E-04   3.16754E+01
CO2(aq)                              CO2(aq)  2.09764E-04   6.09047E-04   2.903         7.29332E-05   1.87795E-04   8.26481E+00
NpO2+                                NpO2+    5.08524E-05   1.01192E-04   1.990         1.76809E-05   4.55264E-05   1.22488E+01   -1.03E-10
CO3=                                 CO3=     3.72976E-07   9.68700E-09   2.5972E-02    1.29680E-07   3.33913E-07   2.00178E-02    1.16E-10
H+                                   H+       2.58815E-07   1.01481E-06   3.921         8.99877E-08   2.31708E-07   2.33539E-04   -1.00E-10
NpO2CO3-                             NpO2CO3- 1.33591E-07   2.43057E-07   1.819         4.64684E-08   1.19600E-07   3.93550E-02    4.94E-14
OH-                                  OH-      1.42122E-08   7.72597E-09   0.5436        4.94146E-09   1.27237E-08   2.16396E-04    1.02E-10
NpO2OH(aq)                           NpO2OH(aq) 3.01827E-10  3.01827E-10   1.000         1.04943E-10   2.70216E-10   7.72964E-05   -2.15E-11
NpO2(CO3)2=-                         NpO2(CO3)2=- 2.39199E-10  6.19242E-15  2.5888E-05    8.31675E-11   2.14147E-10   8.33172E-05    1.24E-10
NpO2(CO3)3=3-                        NpO2(CO3)3=3- 1.81516E-14  1.43695E-23  7.9155E-10    6.31186E-15   1.62521E-14   7.29851E-09   -3.61E-07
NpO2(OH)2-                           NpO2(OH)2-   3.76182E-16  1.12470E-16  0.2988        1.30865E-16   3.36962E-16   1.02120E-10    8.05E-11
HCl(aq).....to.titrate.acid.only     0.00000E+00  0.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.45E+02
NaOH(aq)...to.titrate.base.only      0.00000E+00  0.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+02
NpO2OH(aged)_____________NpO2OH(aged)  0.00000E+00  1.00000E+00  1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.79E+00
NpO2OH(amor)_____________NpO2OH(amor)  0.00000E+00  1.00000E+00  1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.39E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED   0.00000E+00  1.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.35E+02
NaCl_____________________Halite      0.00000E+00  1.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3___________________Nahcolite   0.00000E+00  1.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.56E+00
Na2CO3.10H2O_____________Natron      0.00000E+00  1.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -6.03E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate   0.00000E+00  1.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -6.87E+00
Na2CO3.H2O_____________Thermonatrite 0.00000E+00  1.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.16E+00
Na3H(CO3)2.2H2O_____________Trona    0.00000E+00  1.00000E+00  1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.68E+00

pH (-log(aH+)); pmH(-log(mH+))          5.9936        6.5870
Osmotic Coefficient=     1.241681
Equilibrium RH (%) =    77.803013
Ionic Strength (m) =     5.610081
Density, kg/m3     =     1188.83
fCO2(g); log[fCO2(g)]=                                1.847E-02     -1.73

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -4.63662770E+01
Flashing Titration #          4
# inversions for batch pblm          25
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                    FMT V2.3
 DATABASE:  HNW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFP94)
     Pressure=      1.00000E+00 (=) ATM      Temperature=      2.98E+02 (=) Kelvin

 Elemental Abundances for Flash Problem

   Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

   3.86017335E+01    1.11018070E+02    9.93910555E+01    1.00176245E+05  Hydrogen
   3.66796374E+01    5.55111448E+01    4.96974167E+01    7.95128849E+05  Oxygen
   5.42624556E+00    5.61000927E+00    5.02246836E+00    1.15465392E+05  Sodium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
   1.95040028E+00    5.60932515E+00    5.02185589E+00    1.78039857E+05  Chlorine
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
   3.47590431E+00    8.53880242E-04    7.64526458E-04    9.18184087E+00  Carbon
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Neglon
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Th(IV)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
   3.47561578E+00    2.40650545E-05    2.15447014E-05    5.10713269E+00  Np(V)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
  -2.03919321E-15   -5.86469247E-15   -5.25047836E-15    0.00000000E+00  Charge

   Solution Parameters, Calculated
     SOLUTION MASS      461.718525701536        grams
     H2O MASS           347.706761264890        grams
     TDS(g/kg)          327.896311310982        g/kgH2O

   Specified Solution Density
     DENSITY            1188.82463250872        kg/m^3 = g/l

   Solution Parameters Based on Specified Density
     SOLUTION VOL     0.388382367824256         liters
     TDS                293.555459469871        g/l

   Density based on TDS and NaCl solutions     1188.82463250872      g/l
   Percent relative error vs NaCl density    0.0000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                  WATER    8.31854E-01   7.78037E-01   0.9353        1.93007E+01   4.96952E+01   8.95269E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)        9.99580E+00   1.00000E+00   1.000         3.47561E+00   8.94893E+00   3.15044E+06
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
Na+                                   Na+          5.61001E+00   5.29054E+00   0.9431      1.95064E+00   5.02247E+00   1.15465E+05
Cl-                                   Cl-          5.60933E+00   5.29050E+00   0.9432      1.95040E+00   5.02186E+00   1.78040E+05
HCO3-                                 HCO3-        7.06447E-04   2.61569E-04   0.3703      2.45636E-04   6.32460E-04   3.85909E+01
CO2(aq)                               CO2(aq)      1.46506E-04   4.25377E-04   2.903       5.09412E-05   1.31162E-04   5.77243E+00
NpO2+                                 NpO2+        2.33307E-05   4.76176E-05   1.990       8.32087E-06   2.14244E-05   5.76418E+00   -1.33E-08
CO3=                                  CO3=         7.92644E-07   2.058695-08   2.5972E-02  2.75606E-07   7.09630E-07   4.25843E-02   -7.84E-08
H+                                    H+           1.48381E-07   5.81763E-07   3.921       5.15932E-08   1.32841E-07   4.33891E-04   5.22E-06
NpO2CO3-                              NpO2CO3-     1.33598E-07   2.43069E-07   1.819       4.64529E-08   1.19606E-07   3.93572E-02   1.30E-12
OH-                                   OH-          2.47909E-08   1.34770E-08   0.5436      8.61996E-09   2.21945E-08   3.77469E-04   -5.14E-08
NpO2(CO3)2=-                          NpO2(CO3)2=- 5.08355E-10   1.31608E-14   2.5889E-05  1.76758E-10   4.55114E-10   1.77069E-04   -6.65E-08
NpO2OH(aq)                            NpO2OH(aq)   2.47753E-10   2.47753E-10   1.000       8.61455E-11   2.21806E-10   6.34485E-05   1.52E-08
NpO2(CO3)3=5-                         NpO2(CO3)3=- 8.19789E-14   6.49034E-23   7.9171E-10  2.85046E-14   7.33932E-14   3.29590E-08   -1.33E-07
NpO2(OH)2-                            NpO2(OH)2-   5.38926E-16   1.61042E-16   0.2988      1.87388E-16   4.82683E-16   1.46222E-10   -3.61E-08
HCl(aq).....to.titrate.acid.only      H+Cl-        0.00000E+00   0.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.46E+02
NaOH(aq).....to.titrate.base.only     Na+OH-       0.00000E+00   0.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+02
NpO2OH(aged)_____NpO2OH(aged)         NpO2OH(aged) 0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.88E+00
NpO2OH(amor)_____NpO2OH(amor)         NpO2OH(amor) 0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.47E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED    Na3NpO2(CO3) 0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -9.35E+02
NaCl_____Halite                       NaCl         0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3_____Nahcolite                  NaHCO3       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.46E+00
Na2CO3.10H2O_____Natron               Na2CO3       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -6.50E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate    Na2CO3       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -6.54E+00
Na2CO3.H2O_____Thermonatrite          Na2CO3       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -6.83E+00
Na3H(CO3)2.2H2O_____Trona             Na3H(CO3)    0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -8.27E+00

pH (-log[aH+]); pmH(-log[mH+])                     6.2353        6.8286
Osmotic Coefficient=    1.341856
Equilibrium RH (%) =   77.803683
Ionic Strength (m) =    5.610034
Density, kg/m3     =    1188.82
fCO2(g); log[fCO2(g)]=                                        1.298E-02     -1.89

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=     -4.63672945E+03
Flashing Titration #            5
# inversions for batch pbln          24
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                    FMT V2.3
 DATABASE:  HMW84/PM86; Np(V)-Na-CO3-OH-Cl-ClO4 (HR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=      1.00000E+00 (=) ATM      Temperature=      2.98E+02 (=) Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

  3.86037355E+01    1.11018238E+02    9.93913729E+01    1.00176565E+05  Hydrogen
  3.66807466E+01    5.55114537E+01    4.96977765E+01    7.95134606E+05  Oxygen
  5.42634673E+00    5.61000048E+00    5.02246951E+00    1.15465405E+05  Sodium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Potassium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Magnesium
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Calcium
  1.95042932E+00    5.60912626E+00    5.02168625E+00    1.78033842E+05  Chlorine
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Sulfur
  3.47594038E+00    9.40263760E-04    8.41790570E-04    1.01107465E+01  Carbon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  PosIon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  NegIon
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Air
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Boron
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Bromine
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  TracerEl
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Th(IV)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Am(III)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  U(VI)
  3.47561578E+00    6.76867210E-06    6.05979361E-06    1.43646117E-04  Np(V)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  ClO4-(EL)
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Phosphorus
  0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00  Electron
 -1.79306634E-15   -5.15657522E-15   -4.61653057E-15    0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS       461.719961235951      grams
    H2O MASS            347.724266711458      grams
    TDS(g/Kg)           327.891106372229      g/kgH2O

  Specified Solution Density
    DENSITY             1188.82196527081      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.388401270101675        liters
    TDS              393.551291669683         g/l

  Density based on TDS and NaCl solutions     1188.82196527081      g/l
  Percent relative error vs NaCl density      0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

H2O                                   WATER   8.31855E-01   7.78044E-01   0.9353      1.93017E+01   4.96953E+01   8.95271E+05
Na3NpO2CO3(s)_____Na3NpO2CO3(s)       Na3NpO2CO3(  9.89531E+00   1.00000E+00   1.000       3.47561E+00   8.94851E+00   3.15029E+06
Na+                                   Na+          5.61000E+00   5.29023E+00   0.9430      1.95073E+00   5.02247E+00   1.15465E+05
Cl-                                   Cl-          5.60913E+00   5.29028E+00   0.9432      1.95043E+00   5.02169E+00   1.78034E+05
HCO3-                                 HCO3-        8.74979E-04   3.23972E-04   0.3703      3.04225E-04   7.83343E-04   4.77923E+01
CO2(aq)                               CO2(aq)      6.22872E-05   1.80849E-04   2.903       2.16588E-05   5.57639E-05   2.45416E+00
NpO2+                                 NpO2+        6.63303E-06   1.31976E-05   1.990       2.30647E-06   5.93836E-06   1.59770E+00   -4.41E-08
CO3=                                  CO3=         2.86004E-06   7.42826E-08   2.5973E-02  9.94507E-07   2.56051E-06   1.53654E-01   -4.94E-08
NpO2CO3-                              NpO2CO3-     1.33606E-07   2.43083E-07   1.819       4.64560E-08   1.19613E-07   3.93595E-02   9.87E-13
OH-                                   OH-          7.22202E-08   3.92620E-08   0.5436      2.51127E-08   6.46566E-08   1.09963E-03   -5.99E-09
H+                                    H+           5.09374E-08   1.99697E-07   3.920       1.77122E-08   4.56027E-08   4.59630E-05   5.87E-09
NpO2(CO3)2=-                          NpO2(CO3)2=- 1.83431E-09   4.74903E-14   2.5890E-05  6.37833E-10   1.64220E-09   6.38924E-04   -6.36E-09
NpO2OH(aq)                            NpO2OH(aq)   2.00045E-10   2.00045E-10   1.000       6.95604E-11   1.79096E-10   5.12306E-05   7.57E-10
NpO2(CO3)3=5-                         NpO2(CO3)3=- 1.06720E-12   8.45057E-22   7.9184E-10  3.71092E-13   9.55434E-13   4.29061E-07   -1.27E-08
NpO2(OH)2-                            NpO2(OH)2-   1.26769E-15   3.78813E-16   0.2988      4.40807E-16   1.13493E-15   3.43953E-10   -4.84E-09
HCl(aq).....to.titrate.acid.only      H+Cl-        0.00000E+00   0.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.46E+02
NaOH(aq).....to.titrate.base.only     Na+OH-       0.00000E+00   0.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.97E+02
NpO2OH(aged)_____NpO2OH(aged)         NpO2OH(aged) 0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.97E+00
NpO2OH(amor)_____NpO2OH(amor)         NpO2OH(amor) 0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.56E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED    Na3NpO2(CO3) 0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -9.34E+02
NaCl_____Halite                       NaCl         0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3_____Nahcolite                  NaHCO3       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.36E+00
Na2CO3.10H2O_____Natron               Na2CO3       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -5.95E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate    Na2CO3       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -5.99E+00
Na2CO3.H2O_____Thermonatrite          Na2CO3       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -6.27E+00
Na3H(CO3)2.2H2O_____Trona             Na3H(CO3)    0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00   0.00000E+00   -7.62E+00
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
pH (-log[aH+]); pmH(-log[mH+])      6.6996      7.2930
Osmotic Coefficient=     1.241627
Equilibrium RH (%) =    77.804379
Ionic Strength (m) =     5.610010
Density, kg/m3     =     1188.82
fCO2(g); log[fCO2(g)]=                                  5.484E-03    -2.26

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.63484576E+03
Flashing Titration #          6
# inversions for batch pblm          20
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.86060468E+01   1.11018357E+02   9.93915462E+01   1.00176739E+05  Hydrogen
  3.66820272E+01   5.55118406E+01   4.96981566E+01   7.95140687E+05  Oxygen
  5.42646353E+00   5.61000023E+00   5.02247206E+00   1.15465478E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95046283E+00   5.60889284E+00   5.02148065E+00   1.78026553E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47598202E+00   1.05368461E-03   9.43333564E-04   1.13303794E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerE1
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   5.04774935E-07   4.51910500E-07   1.07124571E-01  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Cl04-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.03443207E-15  -2.97468811E-15  -2.66315282E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      461.766386062029      grams
    H2O MASS           347.744713769081      grams
    TDS(g/kg)          327.889016793691      g/kgH2O

  Specified Solution Density
    DENSITY            1188.82089447700      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388423847702623        liters
    TDS             393.549618457625         g/l

  Density based on TDS and NaCl solutions     1188.82089447700      g/l
  Percent relative error vs NaCl density      0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality     Activity     Act Coef     Total Moles   Molarity     mg/liter     Descriptor

H2O                                WATER      8.31857E-01  7.78050E-01  0.9353       1.93029E+01   4.96953E+01  8.95271E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)        9.99473E+00  1.00000E+00  1.000        3.47562E+00   8.94600E+00  1.15011E+06
Na+                                Na+        5.61000E+00  5.29000E+00  0.9430       1.95085E+00   5.02247E+00  1.15465E+05
Cl-                                Cl-        5.60889E+00  5.26999E+00  0.9431       1.95046E+00   5.02148E+00  1.78027E+05
HCO3-                              HCO3-      9.92658E-04  1.67542E-04  0.3703       3.45192E-04   8.88699E-04  5.42258E+01
CO3=                               CO3=       5.67805E-05  1.47473E-06  2.5972E-02   1.97451E-05   5.08340E-05  3.05050E+00
CO2(aq)                            CO2(aq)    4.03803E-06  1.17243E-05  2.903        1.40420E-06   3.61513E-06  1.59101E-01  -4.22E-08
OH-                                OH-        1.26379E-06  6.87070E-07  0.5437       4.39476E-07   1.13143E-06  1.92426E-02  -9.05E-08
NpO2+                              NpO2+      3.34150E-07  6.64800E-07  1.990        1.16199E-07   2.99155E-07  8.04868E-02   1.77E-07
NpO2CO3-                           NpO2CO3-   1.33613E-07  2.43094E-07  1.819        4.64631E-08   1.19620E-07  3.93616E-02   3.39E-13
NpO2(CO3)2=-                       NpO2(CO3)2=-  3.64151E-08  9.42862E-13  2.5892E-05  1.26632E-08   3.26014E-08  1.26841E-02  -1.13E-07
H+                                 H+         2.91107E-09  1.14116E-08  3.920        1.01231E-09   2.60620E-09  2.62679E-06   1.24E-07
NpO2(CO3)3---                      NpO2(CO3)3---  4.20537E-10  3.33083E-19  7.9204E-10  1.46239E-10  3.76494E-10  1.69074E-04  -2.13E-07
NpO2OH(aq)                         NpO2OH(aq) 1.76340E-10  1.76340E-10  1.000        6.13212E-11   1.57872E-10  4.51599E-05  -2.03E-08
NpO2(OH)2-                         NpO2(OH)2- 1.95555E-14  5.84354E-15  0.2988       6.80031E-15   1.75074E-14  5.30583E-09  -1.48E-07
HCl(aq).....to.titrate.acid.only               0.00000E+00  0.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -2.47E+02
NaOH(aq).....to.titrate.base.only              0.00000E+00  0.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -2.96E+02
NpO2OH(aged)_____________NpO2OH(aged)          0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -3.03E+00
NpO2OH(amor)_____________NpO2OH(amor)          0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -3.62E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED             0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -9.33E+02
NaCl_____________________________Halite        0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -1.23E-01
NaHCO3___________________________Nahcolite     0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -2.31E+00
Na2CO3.10H2O_____________________Natron        0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -4.65E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate             0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -4.69E+00
Na2CO3.H2O_____Thermonatrite                   0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -4.98E+00
Na3H(CO3)2.2H2O__________Trona                 0.00000E+00  1.00000E+00  1.000        0.00000E+00   0.00000E+00  0.00000E+00  -6.27E+00

pH (-log[aH+]); pmH(-log[mH+])      7.9427      8.5359
Osmotic Coefficient=     1.241601
Equilibrium RH (%) =    77.805007
Ionic Strength (m) =     5.610057
Density, kg/m3     =     1188.82
fCO2(g); log[fCO2(g)]=                                  3.555E-04    -3.45

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -4.63497996E+03
Flashing Titration #          7
# inversions for batch pblm          21
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.3
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

	Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
	3.86077395E+01	1.11018365E+02	9.93915827E+01	1.00176776E+05	Hydrogen
	3.66829651E+01	5.55121073E+01	4.96984096E+01	7.95144735E+05	Oxygen
	5.42654906E+00	5.61000051E+00	5.02247378E+00	1.15465517E+05	Sodium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
	1.95048738E+00	5.60871794E+00	5.02123553E+00	1.78021054E+05	Chlorine
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
	3.47601251E+00	1.14118308E-01	1.02166873E-01	1.22713631E+01	Carbon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
	3.47561578E+00	3.61660997E-07	3.23784797E-07	7.67526032E-02	Np(V)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4-(EL)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
	-1.71147437E-15	-4.92142480E-15	-4.40601154E-15	0.00000000E+00	Charge

Solution Parameters, Calculated

SOLUTION MASS	461.786282369672	grams
H2O MASS	347.759934523067	grams
TDS(g/kg)	327.888110523674	g/kgH2O

Specified Solution Density

DENSITY	1188.82043006313	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	0.388440735616523	liters
TDS	293.548892768897	g/l

Density based on TDS and NaCl solutions 1188.82043006313 g/l
Percent relative error vs NaCl density 0.000000000000000E+000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31858E-01	7.78054E-01	0.9353	1.93037E+01	4.96953E+01	8.95272E+05	
NaNpO2CO3(s)	NaNpO2CO3(s)	9.99430E+00	1.00000E+00	1.000	3.47562E+00	8.94761E+00	3.14997E+06	
Na+	Na+	5.61000E+00	5.28994E+00	0.9429	1.95093E+00	5.02247E+00	1.15466E+05	
Cl-	Cl-	5.60872E+00	5.28973E+00	0.9431	1.95049E+00	5.02133E+00	1.78021E+05	
HCO3-	HCO3-	9.99205E-04	3.69960E-04	0.3703	3.47484E-04	8.94560E-04	5.45835E+01	
CO3=	CO3=	1.39997E-04	3.63604E-06	2.5972E-02	4.86855E-05	1.25336E-04	7.52130E+00	
OH-	OH-	3.09556E-06	1.66295E-06	0.5437	1.07651E-06	2.77137E-06	4.71335E-02	-2.35E-08
CO2(aq)	CO2(aq)	1.65938E-06	4.81799E-06	2.903	5.77065E-07	1.48559E-06	6.53807E-02	-1.74E-08
NpO2+	NpO2+	1.35537E-07	2.69637E-07	1.989	4.71342E-08	1.21342E-07	3.26468E-02	3.22E-09
NpO2CO3-	NpO2CO3-	1.33616E-07	2.43097E-07	1.819	4.64663E-08	1.19623E-07	3.93626E-02	9.94E-13
NpO2(CO3)2=-	NpO2(CO3)2=-	8.97771E-08	2.32472E-12	2.5894E-05	3.12209E-08	8.03749E-08	3.12711E-02	-3.53E-09
NpO2(CO3)3=5-	NpO2(CO3)3=5-	2.55580E-09	2.02485E-18	7.9225E-10	8.88807E-10	2.28814E-09	1.02755E-03	-8.03E-09
H+	H+	1.18855E-09	4.65884E-09	3.920	4.13329E-10	1.06407E-09	1.07248E-06	6.85E-09
NpO2OH(aq)	NpO2OH(aq)	1.75190E-10	1.75190E-10	1.000	6.09240E-11	1.56842E-10	4.48655E-05	-2.80E-09
NpO2(OH)2-	NpO2(OH)2-	4.75887E-14	1.42202E-14	0.2988	1.65494E-14	4.26048E-14	1.29119E-08	-9.66E-09
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.96E+02
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.62E+00
Na3NpO2(CO3)2(s)_DISABLED	_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.32E+02
NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.34E-01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.31E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.36E+00
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.30E+00
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.58E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.87E+00

pH (-log[aH+]); pnH(-log[nH+]) 8.3317 8.9250
Osmotic Coefficient= 1.241589
Equilibrium RH (%) = 77.805353
Ionic Strength (m) = 5.610141
Density, kg/m3 = 1188.82
fCO2(g); log[fCO2(g)]= 1.461E-04 -3.84

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -4.63507818E+03
Flashing Titration # 8
inversions for batch pblm 21
1Benchmark TITRATE Problem: Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
DATABASE: NOM84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,PRF90,P91,RPFR92,RFF94,RRFF94)
Pressure= 1.00000E+00 [*] ATM Temperature= 2.98E+02 [*] Kelvin

Elemental Abundances for Flash Problem

	Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
	3.86097415E+01	1.11018371E+02	9.93916217E+01	1.00176815E+05	Hydrogen
	3.66840743E+01	5.55124212E+01	4.96987076E+01	7.95149502E+05	Oxygen
	5.42665023E+00	5.61000082E+00	5.02247577E+00	1.15465563E+05	Sodium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
	1.95051642E+00	5.60851089E+00	5.02114187E+00	1.78014543E+05	Chlorine
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
	3.47604858E+00	1.24484251E-03	1.11447244E-03	1.33859285E-01	Carbon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
	3.47561578E+00	3.74514610E-07	3.35292385E-07	7.94804563E-02	Np(V)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4-(EL)
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
	-1.31010731E-15	-3.76707986E-15	-3.37256052E-15	0.00000000E+00	Charge

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
  Solution Parameters, Calculated
    SOLUTION MASS      461.8098366671?1       grams
    H2O MASS           347.779949659092       grams
    TDS(g/kg)          327.887052988433       g/kgH2O

  Specified Solution Density
    DENSITY            1188.81988813375       kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388660725864989         liters
    TDS             293.548045955388          g/l

  Density based on TDS and NaCl solutions     1188.81988813375      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality     Activity     Act Coef     Total Moles    Molarity     mg/liter     Descriptor
H2O                                  WATER    8.31859E-01  7.78058E-01  0.9353       1.93047E+01    4.96954E+01  8.95272E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)         9.99378E+00  1.00000E+00   1.000       3.47562E+00    8.94715E+00  3.14981E+06
Na+                                  Na+      5.61000E+00  5.28987E+00  0.9429       1.95103E+00    5.02148E+00  1.15466E+05
Cl-                                  Cl-      5.60851E+00  5.28943E+00  0.9431       1.95052E+00    5.02114E+00  1.78015E+05
HCO3-                                HCO3-    1.00274E-03  3.71260E-04  0.3702       3.48729E-04    8.97721E-04  5.47764E+01
CO3=                                 CO3=     2.40670E-04  6.25064E-06  2.5972E-02   8.36995E-05    2.15465E-04  1.29299E+01
OH-                                  OH-      5.30281E-06  2.88301E-06  0.5437       1.84420E-06    4.74746E-06  8.07415E-02  -2.62E-07
CO2(aq)                              CO2(aq)  9.72059E-07  2.82237E-06   2.903       3.38061E-07    8.70257E-07  3.82998E-02  -2.79E-07
NpO2(CO3)2=-                         NpO2(CO3)2=-  1.54320E-07  3.99643E-12  2.5897E-05  5.36690E-08  1.38158E-07  5.37525E-02  1.94E-08
NpO2CO3-                             NpO2CO3-  1.33620E-07  2.43100E-07   1.819       4.64701E-08    1.19626E-07  3.93638E-02  1.72E-11
NpO2+                                NpO2+    7.88495E-08  1.56851E-07   1.989       2.74221E-08    7.05917E-08  1.89925E-02  -1.38E-08
NpO2(CO3)3=5-                        NpO2(CO3)3=5-  7.55070E-09  5.98397E-18  7.9251E-10  2.62597E-09  6.75993E-09  3.03571E-03  1.34E-08
H+                                   H+       6.93877E-10  2.71860E-09   3.919       2.41315E-10    6.21208E-10  6.26116E-07  2.77E-08
NpO2OH(aq)                           NpO2OH(aq)  1.74579E-10  1.74579E-10  1.000      6.07148E-11    1.56296E-10  4.47092E-05  -3.42E-08
NpO2(OH)2-                           NpO2(OH)2-  8.12402E-14  2.42753E-14  0.2988     2.82535E-14    7.27120E-14  2.20421E-08  -6.38E-08
HCl(aq).....to.titrate.acid.only     0.00000E+00  0.00000E+00  1.000      0.00000E+00    0.00000E+00  0.00000E+00  -2.48E+02
NaOH(aq).....to.titrate.base.only    0.00000E+00  0.00000E+00  1.000      0.00000E+00    0.00000E+00  0.00000E+00  -2.95E+02
NpO2OH(aged)_____________NpO2OH(aged)  0.00000E+00  1.00000E+00  1.000     0.00000E+00    0.00000E+00  0.00000E+00  -3.03E+00
NpO2OH(amor)_____________NpO2OH(amor)  0.00000E+00  1.00000E+00  1.000     0.00000E+00    0.00000E+00  0.00000E+00  -3.62E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED  0.00000E+00  1.00000E+00  1.000      0.00000E+00    0.00000E+00  0.00000E+00  -9.32E+02
NaCl_____________________Halite      0.00000E+00  1.00000E+00  1.000      0.00000E+00    0.00000E+00  0.00000E+00  -1.24E-01
NaHCO3_____________________Nahcolite  0.00000E+00  1.00000E+00  1.000     0.00000E+00    0.00000E+00  0.00000E+00  -2.30E+00
Na2CO3.10H2O_____________Natron      0.00000E+00  1.00000E+00  1.000      0.00000E+00    0.00000E+00  0.00000E+00  -4.02E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate   0.00000E+00  1.00000E+00  1.000      0.00000E+00    0.00000E+00  0.00000E+00  -4.06E+00
Na2CO3.H2O_____Thermonatrite         0.00000E+00  1.00000E+00  1.000      0.00000E+00    0.00000E+00  0.00000E+00  -4.35E+00
Na3H(CO3)2.2H2O_____________Trona    0.00000E+00  1.00000E+00  1.000      0.00000E+00    0.00000E+00  0.00000E+00  -5.64E+00

pH (-log{aH+}); pmH(-log{mH+})       8.5655       9.1587
Osmotic Coefficient=    1.241574
Equilibrium RH (%) =   77.805756
Ionic Strength (m) =    5.610242
Density, kg/m3     =    1188.82
fCO2(g); log{fCO2(g)}=                                  8.559E-05    -4.07

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -6.63519432E+03
Flashing Titration #          9
# inversions for batch pbim          22
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.6imolal NaCl                FMT V2.3
DATABASE:  HMNB4/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,PRP90,P91,RFFR92,RFF94,RRFF96)
   Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

  3.86117435E+01   1.11018376E+02   9.93916598E+01   1.00176854E+05  Hydrogen
  3.66851835E+01   5.55127348E+01   4.96990052E+01   7.95154264E+05  Oxygen
  5.42675140E+00   5.61000112E+00   5.02247774E+00   1.15465608E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95054545E+00   5.60830381E+00   5.02095819E+00   1.78008031E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47608466E+00   1.34652749E-01   1.20729916E-03   1.45008694E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   4.23669533E-07   3.79299532E-07   8.99122713E-02  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.32066722E-15  -1.79724708E-15  -1.39956954E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      461.833395409572       grams
    H2O MASS           347.795967332738       grams
    TDS(g/kg)          327.885998692483       g/kgH2O

  Specified Solution Density
    DENSITY            1188.81934786396       kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388480719328282         liters
    TDS             293.547201735043          g/l

  Density based on TDS and NaCl solutions     1188.81934786396      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality     Activity     Act Coef     Total Moles    Molarity     mg/liter     Descriptor
H2O                                  WATER    8.31861E-01  7.78062E-01  0.9353       1.93057E+01    4.96954E+01  8.95272E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)         9.99326E+00  1.00000E+00   1.000       3.47562E+00    8.94669E+00  3.14965E+06
Na+                                  Na+      5.61000E+00  5.28981E+00  0.9429       1.95114E+00    5.02148E+00  1.15466E+05
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
1355 Cl-                                Cl-      5.60830E+00   5.28912E+00   0.9431     1.95055E+00   5.02096E+00   1.78008E+05
1356 HCO3-                              HCO3-    1.00546E-03   3.72261E-04   0.3702     3.49695E-04   9.00160E-04   5.49251E+01
1357 CO3=                               CO3=     3.41763E-04   8.87612E-06   2.5972E-02 1.18864E-04   3.05971E-04   1.83610E+01
1358 OH-                                OH-      7.50984E-06   4.08299E-06   0.5437     2.61189E-06   6.72335E-06   1.14346E-01   -7.54E-09
1359 CO2(aq)                            CO2(aq)  6.88224E-07   1.99826E-06   2.904      2.39361E-07   6.16147E-07   2.71165E-02   -3.37E-08
1360 NpO2(CO3)2=-                       NpO2(CO3)2=-  2.19119E-07   5.67513E-12   2.5900E-05 7.62086E-08   1.96171E-07   7.63233E-02   1.61E-08
1361 NpO2CO3-                           NpO2CO3- 1.33624E-07   2.43103E-07   1.819      4.64739E-08   1.19630E-07   3.93649E-02   1.56E-12
1362 NpO2+                              NpO2+    5.55311E-08   1.10457E-07   1.989      1.93136E-08   4.97156E-08   1.33758E-02   -1.58E-08
1363 NpO2(CO3)3=5-                      NpO2(CO3)3=5- 1.52213E-08   1.20668E-17   7.9276E-10 5.29390E-09   1.36272E-08   6.11963E-03   3.15E-08
1364 H+                                 H+       4.89995E-10   1.92033E-09   3.919      1.70418E-10   4.38679E-10   4.42145E-07   -1.98E-08
1365 NpO2OH(aq)                         NpO2OH(aq) 1.74113E-10   1.74113E-10   1.000      6.05558E-11   1.55879E-10   4.45898E-05   4.15E-09
1366 NpO2(OH)2-                         NpO2(OH)2- 1.14749E-13   3.42875E-14   0.2988     3.99092E-14   1.02731E-13   3.11339E-08   2.40E-08
1367 HCl(aq).....to.titrate.acid.only   0.00000E+00   0.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -2.48E+02
1368 NaOH(aq).....to.titrate.base.only  0.00000E+00   0.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+02
1369 NpO2OH(aged)_____NpO2OH(aged)      0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.03E+00
1370 NpO2OH(amor)_____NpO2OH(amor)      0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.63E+00
1371 Na3NpO2(CO3)2(s)_DISABLED_DISABLED 0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -9.32E+02
1372 NaCl_____Halite                    0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
1373 NaHCO3_____Nahcolite               0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -2.30E+00
1374 Na2CO3.10H2O_____Natron            0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.87E+00
1375 Na2CO3.7H2O____Na2CO3-Heptahydrate 0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -1.91E+00
1376 Na2CO3.H2O_____Thermonatrite       0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -4.20E+00
1377 Na3H(CO3)2.2H2O_____Trona          0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -5.48E+00
1378
1379 pH (-log[aH+]); pmH(-log[mH+])     8.7166        9.3098
1380 Osmotic Coefficient=    1.261560
1381 Equilibrium RH (%) =   77.806158
1382 Ionic Strength (m) =    5.610344
1383 Density, kg/m3     =    1188.82
1384 fCO2(g); log[fCO2(g)]=                                    6.060E-05     -4.22
1385
1386 NOTES:  - Water 'molality' is mole fraction H2O in aqueous phase
1387         - Gas 'molality' and 'activity' are gas partial pressures
1388         - 'Descriptor' means:
1389           'dG/RT/ln10 for species with nonzero concs. (convergence criterion)
1390           'Saturation Index for minerals, SI=log10(IAP/Ksp)
1391           'log10(activity) for aqueous species with very small concentrations
1392           'log10(partial pressure) for gases
1393
1394 Total G/RT=    -4.635310455E+03
1395 Flashing Titration #          10
1396 # inversions for batch pblm    22
1397 1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                    FMT V2.3
1398 DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1399 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
1400     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin
1401
1402 Elemental Abundances for Flash Problem
1403
1404  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
1405
1406  3.86166895E+01   1.11010383E+02   9.93917155E+01   1.00176910E+05  Hydrogen
1407  3.86868157E+01   5.55131962E+01   4.96994431E+01   7.95161269E+04  Oxygen
1408  5.42690026E+00   5.61000156E+00   5.02248064E+00   1.15465675E+05  Sodium
1409  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
1410  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
1411  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
1412  1.95058817E+00   5.60799912E+00   5.02068792E+00   1.77998449E+05  Chlorine
1413  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
1414  3.47613772E+00   1.50110283E-03   1.34389622E-03   1.61415376E+01  Carbon
1415  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
1416  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
1417  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
1418  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
1419  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
1420  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
1421  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
1422  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
1423  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
1424  3.47561578E+00   5.18432642E-07   4.64138535E-07   1.10023204E-01  Np(V)
1425  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
1426  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
1427  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
1428 -1.38030716E-15  -3.96842423E-15  -3.55282145E-15   0.00000000E+00  Charge
1429
1430  Solution Parameters, Calculated
1431    SOLUTION MASS      461.868064846891      grams
1432    H2O MASS           347.822481718624      grams
1433    TDS(g/kg)          327.884450035425      g/kgH2O
1434
1435  Specified Solution Density
1436    DENSITY            1188.81855426012      kg/m^3 = g/l
1437
1438  Solution Parameters Based on Specified Density
1439    SOLUTION VOL    0.388510141595444        liters
1440    TDS             293.545961657349         g/l
1441
1442  Density based on TDS and NaCl solutions    1188.81855426012      g/l
1443  Percent relative error vs NaCl density     0.000000000000000E+000 %
1444
1445
1446
1447 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1448
1449 Species Name                           Molality      Activity      Act Coef   Total Moles   Molarity      mg/liter      Descriptor
1450
1451 H2O                                   WATER    8.31862E-01   7.78067E-01   0.9353     1.93072E+01   4.96956E+01   8.95273E+05
1452 Na2NpO2CO3(s)_____Na2NpO2CO3(s)      9.99250E+00   1.00000E+00   1.000      1.47562E+00   8.94601E+00   3.14941E+06
1453 Na+                                 Na+      5.61000E+00   5.28971E+00   0.9429     1.95128E+00   5.02248E+00   1.15466E+05
1454 Cl-                                 Cl-      5.60800E+00   5.28867E+00   0.9431     1.95059E+00   5.02069E+00   1.77998E+05
1455 HCO3-                               HCO3-    1.00903E-03   3.73572E-04   0.3702     3.50963E-04   9.03356E-04   5.51202E+01
1456 CO3=                                CO3=     4.90734E-04   1.27449E-05   2.5971E-02 1.70688E-04   4.39341E-04   2.63645E+01
1457 OH-                                 OH-      1.07451E-05   5.84210E-06   0.5437     3.73739E-06   9.61980E-06   1.63607E-01   -4.54E-08
1458 CO2(aq)                             CO2(aq)  4.82685E-07   1.40148E-06   2.904      1.67869E-07   4.32135E-07   1.90162E-02   -8.60E-08
1459 NpO2(CO3)2=-                        NpO2(CO3)2=-  3.14582E-07   8.14888E-12   2.5904E-05 1.09419E-07   2.81637E-07   1.09575E-01   2.57E-08
1460 NpO2CO3-                            NpO2CO3- 1.33630E-07   2.43107E-07   1.819      4.64794E-08   1.19635E-07   3.93666E-02   4.38E-12
1461 NpO2+                               NpO2+    3.86794E-08   7.69287E-08   1.989      1.34536E-08   3.46286E-08   9.31671E-03   -2.12E-08
1462 NpO2(CO3)3=5-                       NpO2(CO3)3=5- 3.13678E-08   2.48787E-17   7.9313E-10 1.09104E-08   2.80827E-08   1.26112E-02   6.46E-08
1463 H+                                  H+       3.42501E-10   1.34211E-09   3.919      1.19129E-10   3.06631E-10   3.09054E-07   -2.53E-08
1464 NpO2OH(aq)                          NpO2OH(aq) 1.73507E-10   1.73507E-10   1.000      6.03495E-11   1.55336E-10   4.44344E-05   4.67E-09
1465 NpO2(OH)2-                          NpO2(OH)2- 1.63619E-13   4.88889E-14   0.2988     5.69105E-14   1.46484E-13   4.43936E-08   2.97E-08
1466 HCl(aq).....to.titrate.acid.only    0.00000E+00   0.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -2.48E+02
1467 NaOH(aq).....to.titrate.base.only   0.00000E+00   0.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+02
1468 NpO2OH(aged)_____NpO2OH(aged)       0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.03E+00
1469 NpO2OH(amor)_____NpO2OH(amor)       0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.63E+00
1470 Na3NpO2(CO3)2(s)_DISABLED_DISABLED  0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -9.32E+02
1471 NaCl_____Halite                     0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
1472 NaHCO3_____Nahcolite                0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -2.30E+00
1473 Na2CO3.10H2O_____Natron             0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.71E+00
1474 Na2CO3.7H2O____Na2CO3-Heptahydrate  0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.75E+00
1475 Na2CO3.H2O_____Thermonatrite        0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -4.04E+00
1476 Na3H(CO3)2.2H2O_____Trona           0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -5.33E+00
1477
1478 pH (-log[aH+]); pmH(-log[mH+])      8.8722        9.4653
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
Osmotic Coefficient=    1.241539
Equilibrium RH (%) =   77.806749
Ionic Strength (m) =    5.610494
Density, kg/m3     =    1188.82
fCO2(g); log[fCO2(g)]=                                    4.250E-05    -4.37

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          "Saturation Index for minerals, SI=log10(IAP/Ksp)
          "log10(activity) for aqueous species with very small concentrations
          "log10(partial pressure) for gases

Total G/RT=    -6.63568130E+03
Flashing Titration #        11
# inversions for batch pblm        23
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                  FMT V2.3
DATABASE:  HMW84/PW85; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

 Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter

 3.86270048E+01   1.11018410E+02   9.93919460E+01   1.00177142E+05  Hydrogen
 3.66936389E+01   5.55151238E+01   4.97012721E+01   7.95190533E+05  Oxygen
 5.42752259E+00   5.61000344E+00   5.02249276E+00   1.15465953E+05  Sodium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
 1.95076677E+00   5.60672581E+00   5.01955838E+00   1.77958403E+05  Chlorine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
 3.47635958E+00   2.13879267E-03   1.91480644E-03   2.29987401E+01  Carbon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
 3.47561578E+00   1.02582330E-06   9.18393392E-07   2.17703500E-01  Np(V)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
-1.79974135E-15  -5.17266157E-15  -4.63095175E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS      462.013011582888      grams
   H2O MASS           347.933328203232      grams
   TDS(g/kg)          327.877998836092      g/kgH2O

 Specified Solution Density
   DENSITY            1188.81524635729      kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL     0.388633147146740       liters
   TDS              293.540795885520        g/l

 Density based on TDS and NaCl solutions    1188.81524635729      g/l
 Percent relative error vs NaCl density     0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

 Species Name                          Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor

 H2O                          WATER    8.31870E-01   7.78092E-01   0.9354        1.93133E+01   4.96955E+01   8.95274E+05
 NaNpO2CO3(s)_____NaNpO2CO3(s)         9.98931E+00   1.00000E+00   1.000         3.47562E+00   8.94318E+00   3.14841E+06
 Na+                          Na+      5.61000E+00   5.28932E+00   0.9428        1.95191E+00   5.02249E+00   1.15466E+05
 Cl-                          Cl-      5.60673E+00   5.28679E+00   0.9429        1.95077E+00   5.01956E+00   1.77958E+05
 CO3=                         CO3=     1.31197E-03   2.89290E-05   2.5969E-02    3.87586E-04   9.97306E-04   5.98475E+01
 HCO3-                        HCO3-    1.02256E-03   3.78536E-04   0.3702        3.55784E-04   9.15475E-04   5.58596E+01
 OH-                          OH-      2.40681E-05   1.30872E-05   0.5438        8.37409E-06   2.15475E-05   3.66465E-01   -4.77E-09
 NpO2(CO3)2=-          NpO2(CO3)2=-    7.13640E-07   1.84981E-11   2.5921E-05    2.48299E-07   6.38904E-07   2.48575E-01    9.86E-09
 CO2(aq)                  CO2(aq)      2.18331E-07   6.33934E-07   2.904         7.59645E-08   1.95466E-07   8.60242E-03   -3.55E-08
 NpO2(CO3)3=5-         NpO2(CO3)3=5-   1.61308E-07   1.28190E-16   7.9469E-10    5.61244E-08   1.44415E-07   6.48530E-02    1.95E-08
 NpO2CO3-                  NpO2CO3-    1.33654E-07   2.43125E-07   1.819         4.65026E-08   1.19657E-07   3.93738E-02    1.59E-12
 NpO2+                        NpO2+    1.70496E-08   3.38942E-08   1.988         5.93214E-09   1.52641E-08   4.10676E-03   -9.06E-09
 NpO2OH(aq)            NpO2OH(aq)      1.71249E-10   1.71249E-10   1.000         5.95834E-11   1.53315E-10   4.38565E-05    1.05E-08
 H+                           H+       1.52981E-10   5.99136E-10   3.916         5.32272E-11   1.36960E-10   1.38042E-07   -1.95E-08
 NpO2(OH)2-            NpO2(OH)2-      3.61801E-13   1.08094E-13   0.2988        1.25863E-13   3.23912E-13   9.81651E-08    3.00E-08
 HCl(aq).....to.titrate.acid.only      0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.49E+02
 NaOH(aq).....to.titrate.base.only     0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+02
 NpO2OH(aged)_____NpO2OH(aged)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.04E+00
 NpO2OH(amor)_____NpO2OH(amor)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.63E+00
 Na3NpO2(CO3)2(s)_DISABLED_DISABLED    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.32E+02
 NaCl_____________________Halite       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
 NaHCO3___________________Nahcolite    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.30E+00
 Na2CO3.10H2O_____________Natron       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.36E+00
 Na2CO3.7H2O____Na2CO3-Heptahydrate    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.39E+00
 Na2CO3.H2O_____________Thermonatrite  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.68E+00
 Na3H(CO3)2.2H2O_____________Trona     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.96E+00

 pH (-log[aH+]); pmH(-log[mH+])       9.2225        9.8154
 Osmotic Coefficient=    1.241451
 Equilibrium RH (%) =   77.809217
 Ionic Strength (m) =    5.611121
 Density, kg/m3     =    1188.82
 fCO2(g); log[fCO2(g)]=                                    1.922E-05    -4.72

 NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
         - Gas "molality" and "activity" are gas partial pressures
         - "Descriptor" means:
           "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
           "Saturation Index for minerals, SI=log10(IAP/Ksp)
           "log10(activity) for aqueous species with very small concentrations
           "log10(partial pressure) for gases

 Total G/RT=    -4.63619543E+03
 Flashing Titration #        12
 # inversions for batch pblm        23
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                  FMT V2.3
DATABASE:  HMW84/PW85; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

 Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
 3.86445564E+01  1.11018446E+02  9.93922712E+01  1.00177470E+05  Hydrogen
 3.67033633E+01  5.55178691E+01  4.97038762E+01  7.95232196E+05  Oxygen
 5.42849952E+00  5.61000623E+00  5.02251004E+00  1.15466351E+05  Sodium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
 1.95102131E+00  5.60491244E+00  5.01794968E+00  1.77901370E+05  Chlorine
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
 3.47667577E+00  3.04710993E-03  2.72800778E-03  3.27661005E+01  Carbon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  PosIon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  NegIon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Th(IV)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
 3.47561578E+00  1.94420912E-06  1.74060588E-06  4.12607491E-01  Np(V)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Cl04-(EL)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electron
-1.54424874E-15 -4.43633236E-15 -3.97174671E-15  0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS      462.219610892029      grams
   H2O MASS           348.091309672199      grams
   TDS(g/kg)          327.868860981635      g/KgH2O

 Specified Solution Density
   DENSITY            1188.81056566046      kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL     0.388808464732340       liters
   TDS               393.533478748712       g/l

 Density based on TDS and NaCl solutions     1188.81056566046      g/l
 Percent relative error Vs NaCl density   0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                              Molality      Activity     Act Coef     Total Moles    Molarity     mg/liter     Descriptor
H2O                              WATER    8.31881E-01   7.78127E-01   0.9354      1.93221E+01   4.96957E+01  8.95277E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)    9.98478E+00   1.00000E+00   1.000       3.47562E+00   8.93914E+00  3.14699E+06
Na+                               Na+    5.61001E+00   5.28876E+00   0.9427      1.95279E+00   5.02251E+00  1.15466E+05
Cl-                               Cl-    5.60491E+00   5.28411E+00   0.9428      1.95103E+00   5.01795E+00  1.77901E+05
CO3=                             CO3=    2.00200E-03   5.19855E-05   2.5967E-02  6.96880E-04   1.79235E-03  1.07557E+02
HCO3-                           HCO3-    1.04072E-03   1.05192E-04   0.1011      3.62367E-04   9.31738E-04  5.68519E+01
OH-                               OH-    4.24987E-05   2.31124E-05   0.5438      1.47934E-05   3.80481E-05  6.47095E-01   -6.11E-08
NpO2(CO3)2=-          NpO2(CO3)2=-       1.36136E-06   3.32446E-11   2.5945E-05  4.46030E-07   1.14717E-06  4.46325E-01    4.76E-08
NpO2(CO3)3=5-         NpO2(CO3)3=5-      5.19497E-07   4.13996E-16   7.9692E-10  1.80832E-07   4.65094E-07  2.08862E-01   1.05E-07
NpO2CO3-                    NpO2CO3-     1.33688E-07   2.43151E-07   1.819       4.65356E-08   1.19688E-07  3.93840E-02    1.10E-12
CO2(aq)                     CO2(aq)      1.25799E-07   3.65271E-07   2.904       4.37896E-08   1.12625E-07  4.95661E-03   -3.36E-07
NpO2+                       NpO2+        9.49502E-09   1.88635E-08   1.987       3.30513E-09   8.50067E-09  2.28708E-03   -4.00E-08
NpO2OH(aq)                  NpO2OH(aq)   1.68316E-10   1.68316E-10   1.000       5.85892E-11   1.50689E-10  4.31052E-05    1.03E-07
H+                                H+     8.66958E-11   3.39270E-10   3.913       3.01760E-11   7.76167E-11  7.82299E-08   -1.46E-07
NpO2(OH)2-                  NpO2(OH)2-   6.28103E-13   1.87627E-13   0.2987      2.18637E-13   5.62326E-13  1.70419E-07    2.42E-07
HCl(aq).....to.titrate.acid.only         0.00000E+00   0.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -2.49E+02
NaOH(aq).....to.titrate.base.only        0.00000E+00   0.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -2.94E+02
NpO2OH(aged)_____________NpO2OH(aged)    0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -3.05E+00
NpO2OH(amor)_____________NpO2OH(amor)    0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -3.64E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -9.31E+02
NaCl_____________________Halite          0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -1.24E-01
NaHCO3___________________Nahcolite       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -2.29E+00
Na2CO3.10H2O_____________Natron          0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -3.10E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate       0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -3.16E+00
Na2CO3.H2O_____________Thermonatrite     0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -3.43E+00
Na3H(CO3)2.2H2O_________________Trona     0.00000E+00   1.00000E+00   1.000       0.00000E+00   0.00000E+00  0.00000E+00   -4.70E+00

pH (-log[aH+]); pmH(-log[mH+])          9.4695      10.0620
Osmotic Coefficient=     1.241325
Equilibrium RH (%) =    77.812731
Ionic Strength (m) =     5.612017
Density, kg/m3     =     1188.81
fCO2(g); log[fCO2(g)]=                                1.108E-05    -4.96

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -8.63721297E+03
Flashing Titration #          13
# inversions for batch pblm          29
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.6imolal NaCl                    FMT V2.3
DATABASE:  HMW84/FW88; Np(V)-Na-CO3-OH-Cl-ClO4 (HR96);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFP94,RRFP94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter
 3.87052172E+01  1.11018564E+02  9.93933710E+01  1.00178579E+05  Hydrogen
 3.67369721E+01  5.55273415E+01  4.97128540E+01  7.95175837E+05  Oxygen
 5.43147487E+00  5.61001696E+00  5.02256991E+00  1.15467727E+05  Sodium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
 1.95190103E+00  5.59865735E+00  5.01239980E+00  1.77704610E+05  Chlorine
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
 3.47776859E+00  6.18159604E-03  5.53429668E-03  6.64724375E+01  Carbon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  PosIon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  NegIon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Th(IV)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
 3.47561578E+00  6.66371923E-06  5.96534855E-06  1.41421412E+00  Np(V)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Cl04-(EL)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electron
-1.62237641E-15 -4.65347858E-15 -4.16619444E-15  0.00000000E+00  Charge
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
  Solution Parameters, Calculated
    SOLUTION MASS      462.933837982393      grams
    H2O MASS           348.637344066916      grams
    TDS(g/kg)          327.837782901256      g/kgH2O

  Specified Solution Density
    DENSITY            1188.79461948067      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.389414472952726       liters
    TDS               293.508592654065       g/l

  Density based on TDS and NaCl solutions     1188.79461948067      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality     Activity     Act Coef     Total Moles   Molarity     mg/liter     Descriptor
H2O                                 WATER   8.31919E-01  7.78249E-01  0.9355       1.93524E+01  4.96961E+01  8.95286E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.96914E+00  1.00000E+00   1.000       3.47561E+00  8.92523E+00  3.14209E+06
Na+                                  Na+    5.61002E+00  5.28690E+00  0.9424       1.95586E+00  5.02257E+00  1.15468E+05
Cl-                                  Cl-    5.59866E+00  5.27483E+00  0.9422       1.95190E+00  5.01240E+00  1.77705E+05
CO3=                                 CO3=   5.06639E-03  1.31511E-04  2.5957E-02   1.76633E-03  4.53587E-03  2.72194E+02
HCO3-                                HCO3-  1.09867E-03  4.06390E-04  0.3699       3.83038E-04  9.83625E-04  6.00180E+01
OH-                                  OH-    1.01868E-04  5.54275E-05  0.5441       3.55148E-05  9.12006E-05  1.55108E+00  -1.56E-10
NpO2(CO3)3=4-        NpO2(CO3)3=4-  3.29369E-06  2.65037E-15  8.0468E-10   1.14830E-06  2.94880E-06  1.32423E+00   1.74E-09
NpO2(CO3)2=-         NpO2(CO3)2=-   3.23230E-06  8.41302E-11  2.6028E-05   1.12690E-06  2.89383E-06  1.12589E+00   8.08E-10
NpO2CO3-                NpO2CO3-    1.33806E-07  2.43237E-07   1.818       4.66698E-08  1.19795E-07  3.94192E-02   5.06E-13
CO2(aq)                   CO2(aq)   5.53395E-08  1.60694E-07   2.904       1.92934E-08  4.95446E-08  2.18045E-03  -9.19E-09
NpO2+                       NpO2+   3.76315E-09  7.45927E-09   1.982       1.31197E-09  3.36909E-09  9.06445E-04  -7.94E-10
NpO2OH(aq)             NpO2OH(aq)   1.59617E-10  1.59617E-10   1.000       5.56465E-11  1.42903E-10  4.08780E-05   4.13E-09
H+                                   H+     1.62542E-11  1.41493E-10   1.903       1.26396E-11  3.24578E-11  3.27143E-08  -4.92E-09
NpO2(OH)2-           NpO2(OH)2-     1.42922E-12  4.26707E-13  0.2986       4.98278E-13  1.27956E-12  1.87785E-07   9.06E-09
HCl(aq).....to.titrate.acid.only    0.00000E+00  0.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.49E+02
NaOH(aq)....to.titrate.base.only    0.00000E+00  0.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.94E+02
NpO2OH(aged)_____NpO2OH(aged)       0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.07E+00
NpO2OH(amor)_____NpO2OH(amor)       0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.66E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED  0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -9.31E+02
NaCl_____________________Halite     0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.25E-01
NaHCO3___________________Nahcolite  0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.26E+00
Na2CO3.10H2O_____________Natron     0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.70E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate  0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.74E+00
Na2CO3.H2O_____Thermonatrite        0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.03E+00
Na3H(CO3)2.2H2O_____________Trona   0.00000E+00  1.00000E+00   1.000       0.00000E+00  0.00000E+00  0.00000E+00  -4.28E+00

pH (-log[aH+]); pmH(-log[mH+])      9.8493       10.4406
Osmotic Coefficient=    1.240893
Equilibrium RH (%) =   77.824851
Ionic Strength (m) =    5.615126
Density, kg/m3     =    1188.79
fCO2(g); log[fCO2(g)]=                                  4.873E-06    -5.31

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -4.64072887E+01
Flashing Titration #          14
# inversions for batch pbln          28
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.6lmolal NaCl                    FMT V2.3
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RFFP94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

  Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
 3.89315740E+01  1.11018923E+02  9.93971848E+01  1.00182423E+05  Hydrogen
 3.68623841E+01  5.55624876E+01  4.97460678E+01  7.95907236E+05  Oxygen
 5.44291328E+00  5.61007250E+00  5.02279611E+00  1.15472927E+05  Sodium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Potassium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Magnesium
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Calcium
 1.95518371E+00  5.57548454E+00  4.99182890E+00  1.76975310E+05  Chlorine
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
 3.48184645E+00  1.78114275E-02  1.59468826E-02  1.91538009E+02  Carbon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  PosIon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  NegIon
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Air
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Boron
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Bromine
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  TracerEl
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Tb(IV)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Am(III)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  U(VI)
 3.47561578E+00  4.37689260E-05  3.91870856E-05  9.28922811E+00  Np(V)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  ClO4-(EL)
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Electron
-1.51219098E-15 -4.31222774E-15 -3.86081298E-15  0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      465.601411995302      grams
    H2O MASS           350.675119778128      grams
    TDS(g/kg)          327.728674591707      g/kgH2O

  Specified Solution Density
    DENSITY            1188.73872363963      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.391676827494728       liters
    TDS               293.421219101151       g/l

  Density based on TDS and NaCl solutions     1188.73872363963      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality     Activity     Act Coef     Total Moles   Molarity     mg/liter     Descriptor
H2O                                 WATER   8.32061E-01  7.78697E-01  0.9359       1.94655E+01  4.96979E+01  8.95316E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.91117E+00  1.00000E+00   1.000       3.47560E+00  8.87364E+00  3.12393E+06
Na+                                  Na+    5.61007E+00  5.28057E+00  0.9413       1.96731E+00  5.02280E+00  1.15473E+05
Cl-                                  Cl-    5.57548E+00  5.24002E+00  0.9398       1.95518E+00  4.99183E+00  1.76975E+05
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
CO3=                          CO3=      1.64156E-02   4.25479E-04   2.5920E-02   5.75647E-03   1.46970E-02   8.81954E+02
HCO3-                         HCO3-     1.27533E-03   4.70618E-04   0.3690       4.47227E-04   1.14183E-03   6.96709E+01
OH-                           OH-       2.84255E-04   1.54941E-04   0.5451       9.96810E-05   2.54498E-04   4.32632E+00   -1.39E-09
NpO2(CO3)3=4-     NpO2(CO3)3=4-     3.32871E-05   2.77755E-14   8.3442E-10   1.16730E-05   2.98025E-05   1.33836E+01    5.09E-09
NpO2(CO3)2=2-     NpO2(CO3)2=2-     1.03462E-05   2.72515E-10   2.6339E-05   3.62817E-06   9.26318E-06   3.60398E+00    2.40E-09
NpO2CO3-                NpO2CO3-    1.34242E-07   2.43528E-07    1.814       4.70755E-08   1.20190E-07   3.95491E-02    6.22E-12
CO2(aq)                   CO2(aq)   2.29199E-08   6.65708E-08    2.904       8.03745E-09   2.05206E-08   9.03108E-04   -7.53E-08
NpO2+                       NpO2+   1.17432E-09   2.30834E-09    1.966       4.11806E-10   1.05139E-09   2.82874E-04   -2.44E-09
NpO2OH(aq)            NpO2OH(aq)    1.38078E-10   1.38078E-10    1.000       4.84205E-11   1.23624E-10   3.51611E-05    3.36E-08
H+                            H+    1.31074E-11   5.06456E-11    3.864       4.59644E-12   1.17353E-11   1.16280E-06   -3.61E-08
NpO2(OH)2-            NpO2(OH)2-    3.46327E-12   1.03185E-12    0.2979      1.21448E-12   3.10072E-12   9.39710E-07    6.97E-08
HCl(aq).....to.titrate.acid.only    0.00000E+00   0.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02
NaOH(aq).....to.titrate.base.only   0.00000E+00   0.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+02
NpO2OH(aged)_____________NpO2OH(aged)   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -3.12E+00
NpO2OH(amor)_____________NpO2OH(amor)   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -3.73E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+02
NaCl_____________________Halite   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -1.28E-01
NaHCO3___________________Nahcolite   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -2.20E+00
Na2CO3.10H2O_____________Natron   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -2.19E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -2.23E+00
Na2CO3.H2O_____________Thermonatrite   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+00
Na3H(CO3)2.2H2O_____________Trona   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -3.70E+00

pH (-log[aH+]); pmH(-log[mH+])      10.2955       10.8825
Osmotic Coefficient=    1.239297
Equilibrium RH (%) =   77.869707
Ionic Strength (m) =    5.626852
Density, kg/m3     =    1188.74
fCO2(g); log[fCO2(g)]=                                    2.019E-06    -5.69

NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
        - Gas "molality" and "activity" are gas partial pressures
        - "Descriptor" means:
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=    -4.65384602E+03
Flashing Titration #            15
# inversions for batch pblm            28
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                  FMT V2.3
DATABASE:  HMW84/FWB5; Np(V)-Na-CO3-OH-Cl-ClO4 (HR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FKF90,P91,RFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 (=) ATM      Temperature=     2.98E+02 (=) Kelvin

Elemental Abundances for Flash Problem

  Total Moles       Aq. Molality      Aq. Molarity      Aq. mg/liter

 3.95867206E+01   1.11019649E+02   9.94062599E+01   1.00191569E+05  Hydrogen
 3.72253652E+01   5.56624986E+01   4.98398335E+01   7.97407433E+05  Oxygen
 5.47601956E+00   5.61035435E+00   5.02347422E+00   1.15488517E+05  Sodium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
 1.96468480E+00   5.50989154E+00   4.93352227E+00   1.74908165E+05  Chlorine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
 3.49364905E+00   5.08618173E-02   4.55411352E-02   5.46996977E+02  Carbon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Neglon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
 3.47561578E+00   2.88102498E-04   2.57965074E-04   6.11501564E+01  Np(V)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
-1.39330821E-15  -3.90748680E-15  -3.49873787E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      473.339684533624      grams
    H2O MASS           356.574003417585      grams
    TDS(g/kg)          327.465491025420      g/kgH2O

  Specified Solution Density
    DENSITY            1188.60383111845      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.398231666549673        liters
    TDS                293.210437350980      g/l

  Density based on TDS and NaCl solutions     1188.60383111845      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                          Molality      Activity      Act Coef   Total Moles   Molarity      mg/liter      Descriptor

H2O                          WATER    8.32465E-01   7.79962E-01   0.9369     1.97930E+01   4.97021E+01   8.95393E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)         9.74696E+00   1.00000E+00    1.000     3.47551E+00   8.72736E+00   3.07243E+06
Na+                          Na+      5.61035E+00   5.26665E+00   0.9387     2.00051E+00   5.02347E+00   1.15489E+05
Cl-                          Cl-      5.50989E+00   5.13884E+00   0.9327     1.96468E+00   4.93352E+00   1.74908E+05
CO3=                         CO3=     4.81971E-02   1.24807E-03   2.5788E-02   1.72571E-02   4.33344E-02   2.60046E+03
HCO3-                        HCO3-    1.62010E-03   5.97114E-04   0.3663     5.81251E-04   1.45958E-03   8.90593E+01
OH-                          OH-      6.55397E-04   3.58792E-04   0.5474     2.33698E-04   5.86839E-04   9.98054E+00   -1.51E-09
NpO2(CO3)3=4-     NpO2(CO3)3=4-     2.58546E-04   2.39623E-13   9.2681E-10   9.21906E-05   2.31500E-04   1.03961E+02    2.16E-09
NpO2(CO3)2=2-     NpO2(CO3)2=2-     2.94209E-05   8.01487E-10   2.7242E-05   1.04907E-05   2.63433E-05   1.02493E+01    9.59E-10
NpO2CO3-                NpO2CO3-    1.35468E-07   2.44172E-07    1.802       4.83043E-08   1.21297E-07   3.99135E-02    6.05E-12
CO2(aq)                   CO2(aq)   1.25492E-08   3.64751E-08    2.907       4.47472E-09   1.12365E-08   4.94515E-04   -8.59E-08
NpO2+                       NpO2+   4.11022E-10   7.89015E-10    1.920       1.46560E-10   3.68027E-10   9.90165E-05   -1.06E-09
NpO2OH(aq)            NpO2OH(aq)    1.09291E-10   1.09291E-10    1.000       3.89705E-11   9.78589E-11   2.79929E-05    3.66E-08
NpO2(OH)2-            NpO2(OH)2-    6.38945E-12   1.89128E-12   0.2960     2.27831E-12   5.72107E-12   1.73384E-06    7.43E-08
H+                            H+    5.83272E-12   2.19064E-11    3.756     2.07980E-12   5.22258E-12   5.26384E-09   -3.76E-08
HCl(aq).....to.titrate.acid.only    0.00000E+00   0.00000E+00    1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02
NaOH(aq).....to.titrate.base.only   0.00000E+00   0.00000E+00    1.000     0.00000E+00   0.00000E+00   0.00000E+00   -2.93E+02
NpO2OH(aged)_____________NpO2OH(aged)   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -3.12E+00
NpO2OH(amor)_____________NpO2OH(amor)   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -3.83E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+02
NaCl_____________________Halite   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -1.36E-01
NaHCO3___________________Nahcolite   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -2.10E+00
Na2CO3.10H2O_____________Natron   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -1.72E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -1.76E+00
Na2CO3.H2O_____________Thermonatrite   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -2.05E+00
Na3H(CO3)2.2H2O_____________Trona   0.00000E+00   1.00000E+00   1.000   0.00000E+00   0.00000E+00   0.00000E+00   -3.13E+00

pH (-log[aH+]); pmH(-log[mH+])      10.6596       11.2341
Osmotic Coefficient=    1.234823
```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
1975  Equilibrium RH (%) =   77.996177
1976  Ionic Strength (m) =    5.661425
1977  Density, kg/m3     =    1188.60
1978  fCO2(g), log[fCO2(g)]=                                  1.106E-06    -5.96
1979
1980  NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
1981          - Gas "molality" and "activity" are gas partial pressures
1982          - "Descriptor" means:
1983            "dG/RT/ln10 for species with nonzero concs. (convergence criterion)
1984            "Saturation Index for minerals, SI=log10(IAP/Ksp)
1985            "log10(activity) for aqueous species with very small concentrations
1986            "log10(partial pressure) for gases
1987
1988  Total G/RT=    -4.69179003E+03
1989  TITRATE  file name is U1:[SCSABB.FMT.UM]NP_NACL_BM.TITRATE;2
```

Appendix P: Sample Output File "BATCH_DOC.FOR088"

See Table 16 for explanation of this listing.

```
 1 5.550868155779565E+01 H2O                                  WATER 5.506118174079332E+01
 2 2.016254639034410E-01 Na+                                    Na+ 2.000000000000000E-01
 3 1.008127319517206E-02 K+                                      K+ 1.000000000000001E-02
 4 1.001154090355057E-04 Ca++                                   Ca++ 9.930829876Q7669QE-05
 5 1.098734763517149E-08 Mg++                                   Mg++ 1.089876185025399E-08
 6 3.542680237963029E-08 MgOH+                                MgOH+ 3.514119863014554E-08
 7 1.932115616795198E-13 H+                                      H+ 1.916533289621170E-13
 8 1.108940051468925E-01 Cl-                                     Cl- 1.099999999999999E-01
 9 1.008127119513137E-03 SO4=                                   SO4= 9.999999999596539E-04
10 4.067986529284464E-15 HSO4-                                 HSO4- 4.035191240757798E-15
11 9.879654411868538E-02 OH-                                    OH- 9.800006626742278E-02
12 1.100939975666261E-07 HCO3-                                 HCO3- 1.092064419198057E-07
13 1.000053490322309E-04 CO3=                                   CO3= 9.919912603908383E-05
14 2.211424382613913E-16 CO2(aq)                             CO2(aq) 2.193596324393798E-16
15 6.972356792463450E-07 CaCO3(aq)                         CaCO3(aq) 6.916147055515301E-07
16 5.322055127469460E-11 MgCO3(aq)                         MgCO3(aq) 5.279149790344147E-11
17 1.654105921210009E-11 B(OH)3(aq)                       B(OH)3(aq) 1.640770852239343E-11
18 1.007089477393209E-07 B(OH)4-                             B(OH)4- 9.989705247502938E-08
19 0.000000000000000E+00 B3O3(OH)4-                       B3O3(OH)4- 0.000000000000000E+00
20 0.000000000000000E+00 B4O5(OH)4=                       B4O5(OH)4= 0.000000000000000E+00
21 8.723697139064127E-11 CaB(OH)4+                         CaB(OH)4+ 8.653368448780785E-11
22 6.184659524044248E-15 MgB(OH)4+                         MgB(OH)4+ 6.134836150463729E-15
23 0.000000000000000E+00 Br-                                   Br- 0.000000000000000E+00
24 0.000000000000000E+00 ClO4-                          perchlorate ClO4- 0.000000000000000E+00
25 0.000000000000000E+00 NaOH(aq).....to.titrate.base.only 0.000000000000000E+00
26 0.000000000000000E+00 HCl(aq).....to.titrate.acid.only 0.000000000000000E+00
27 0.000000000000000E+00 HClO4(aq).....to.titrate.acid.only 0.000000000000000E+00
28 0.000000000000000E+00 PosIon.....POSITIVE.ION 0.000000000000000E+00
29 0.000000000000000E+00 NegIon.....NEGATIVE.ION 0.000000000000000E+00
30 0.000000000000000E+00 PosIon(OH)(aq).....to.titrate.base 0.000000000000000E+00
31 0.000000000000000E+00 HNegIon(aq).....to.titrate.acid 0.000000000000000E+00
32 0.000000000000000E+00 Tracer(aq).....conservative.tracer 0.000000000000000E+00
33 0.000000000000000E+00 H3PO4(aq)                         H3PO4(aq) 0.000000000000000E+00
34 0.000000000000000E+00 H2PO4-                             H2PO4- 0.000000000000000E+00
35 0.000000000000000E+00 HPO4=                               HPO4= 0.000000000000000E+00
36 0.000000000000000E+00 PO4=-                               PO4=- 0.000000000000000E+00
37 0.000000000000000E+00 NpO2+                               NpO2+ 0.000000000000000E+00
38 0.000000000000000E+00 NpO2OH(aq)                     NpO2OH(aq) 0.000000000000000E+00
39 0.000000000000000E+00 NpO2(OH)2-                     NpO2(OH)2- 0.000000000000000E+00
40 0.000000000000000E+00 NpO2CO3-                       NpO2CO3- 0.000000000000000E+00
41 0.000000000000000E+00 NpO2(CO3)2=-                 NpO2(CO3)2=- 0.000000000000000E+00
42 0.000000000000000E+00 NpO2(CO3)3=3-                NpO2(CO3)3=3- 0.000000000000000E+00
43 0.000000000000000E+00 Am+++                               Am+++ 0.000000000000000E+00
44 0.000000000000000E+00 AmCO3+                             AmCO3+ 0.000000000000000E+00
45 0.000000000000000E+00 Am(CO3)2-                       Am(CO3)2- 0.000000000000000E+00
46 0.000000000000000E+00 Am(CO3)3=-                     Am(CO3)3=- 0.000000000000000E+00
47 0.000000000000000E+00 Am(OH)2+                       Am(OH)2+ 0.000000000000000E+00
48 0.000000000000000E+00 Am(OH)3(aq)                   Am(OH)3(aq) 0.000000000000000E+00
49 0.000000000000000E+00 Th++++                             Th++++ 0.000000000000000E+00
50 0.000000000000000E+00 UO2++                           U(VI)O2++ 0.000000000000000E+00
51 0.000000000000000E+00 NpO2OH(aged)_____NpO2OH(aged) 0.000000000000000E+00
52 0.000000000000000E+00 NpO2OH(amor)_____NpO2OH(amor) 0.000000000000000E+00
53 0.000000000000000E+00 NaNpO2CO3(s)_____NaNpO2CO3(s) 0.000000000000000E+00
54 0.000000000000000E+00 Na3NpO2(CO3)2(s)_DISABLED_DISABLED 0.000000000000000E+00
55 0.000000000000000E+00 AmOHCO3(c)_____AmOHCO3(c) 0.000000000000000E+00
56 0.000000000000000E+00 Am(OH)3(s)_____Am(OH)3(s) 0.000000000000000E+00
57 0.000000000000000E+00 NaAm(CO3)2.6H2O(c)_____ 0.000000000000000E+00
58 0.000000000000000E+00 AmPO4(c)_____AmPO4(c) 0.000000000000000E+00
59 0.000000000000000E+00 CaSO4_____Anhydrite 0.000000000000000E+00
60 0.000000000000000E+00 NaK3(SO4)2__Aphthitalite/Glaserite 0.000000000000000E+00
61 0.000000000000000E+00 CaCl2.6H2O_____Antarcticite 0.000000000000000E+00
62 0.000000000000000E+00 CaCO3_____Aragonite 0.000000000000000E+00
63 0.000000000000000E+00 K2SO4_____Arcanite 0.000000000000000E+00
64 0.000000000000000E+00 MgCl2.6H2O_____Bischofite 0.000000000000000E+00
65 0.000000000000000E+00 Na2Mg(SO4)2.4H2O_____Bloedite 0.000000000000000E+00
66 1.008080852140455E-03 Mg(OH)2_____Brucite 9.999539072338872E-04
67 0.000000000000000E+00 Na6CO3(SO4)2_____Burkeite 0.000000000000000E+00
68 0.000000000000000E+00 CaCO3_____Calcite 0.000000000000000E+00
69 0.000000000000000E+00 CaCl2.4H2O_____CaCl2_Tetrahydrite 0.000000000000000E+00
70 0.000000000000000E+00 Ca4Cl2(OH)6.13H2O__CaOxychloride A 0.000000000000000E+00
71 0.000000000000000E+00 Ca2Cl2(OH)2.H2O____CaOxychloride B 0.000000000000000E+00
72 0.000000000000000E+00 KMgCl3.6H2O_____Carnallite 0.000000000000000E+00
73 0.000000000000000E+00 MgSO4.7H2O_____Epsomite 0.000000000000000E+00
74 0.000000000000000E+00 CaNa2(CO3)2.5H2O_____Gaylussite 0.000000000000000E+00
75 0.000000000000000E+00 Na2Ca(SO4)2_____Glauberite 0.000000000000000E+00
76 0.000000000000000E+00 CaSO4.2H2O_____Gypsum 0.000000000000000E+00
77 0.000000000000000E+00 NaCl_____Halite 0.000000000000000E+00
78 0.000000000000000E+00 MgSO4.6H2O_____Hexahydrite 0.000000000000000E+00
79 0.000000000000000E+00 KMgClSO4.3H2O_____Kainite 0.000000000000000E+00
80 0.000000000000000E+00 KHCO3_____Kalicinite 0.000000000000000E+00
81 0.000000000000000E+00 MgSO4.H2O_____Kieserite 0.000000000000000E+00
82 0.000000000000000E+00 K2Mg(SO4)2.4H2O_____Leonite 0.000000000000000E+00
83 0.000000000000000E+00 Na4Ca(SO4)3.2H2O_____Labile_Salt 0.000000000000000E+00
84 0.000000000000000E+00 MgCO3_____Magnesite 0.000000000000000E+00
85 0.000000000000000E+00 Mg2Cl(OH)3.4H2O_____MgOxychloride 0.000000000000000E+00
86 0.000000000000000E+00 KHSO4_____Mercallite 0.000000000000000E+00
87 0.000000000000000E+00 Na2SO4.10H2O_____Mirabilite 0.000000000000000E+00
88 0.000000000000000E+00 K8H6(SO4)7_____Misenite 0.000000000000000E+00
89 0.000000000000000E+00 NaHCO3_____Nahcolite 0.000000000000000E+00
90 0.000000000000000E+00 Na2CO3.10H2O_____Natron 0.000000000000000E+00
91 0.000000000000000E+00 MgCO3.3H2O_____Nesquehonite 0.000000000000000E+00
92 0.000000000000000E+00 K2Mg(SO4)2.6H2O Picromerite/Schoen 0.000000000000000E+00
93 0.000000000000000E+00 Na2Ca(CO3)2.2H2O_____Pirssonite 0.000000000000000E+00
94 0.000000000000000E+00 K2MgCa2(SO4)4.2H2O_____Polyhalite 0.000000000000000E+00
95 0.000000000000000E+00 Ca(OH)2_____Portlandite 0.000000000000000E+00
96 0.000000000000000E+00 K2CO3.3/2H2O___Potassium_Carbonate 0.000000000000000E+00
97 0.000000000000000E+00 K8H4(CO3)6.3H2O___K-Sequicarbonate 0.000000000000000E+00
98 0.000000000000000E+00 KNaCO3.6H2O_____K-Na-Carbonate 0.000000000000000E+00
99 0.000000000000000E+00 K2NaH(CO3)2.2H2O___Potassium_Trona 0.000000000000000E+00
100 0.000000000000000E+00 K3H(SO4)2__Sesquipotassium_Sulfate 0.000000000000000E+00
101 0.000000000000000E+00 Na3H(SO4)2____Sesquisodium_Sulfate 0.000000000000000E+00
102 0.000000000000000E+00 Na2CO3.7H2O____Na2CO3-Heptahydrate 0.000000000000000E+00
103 0.000000000000000E+00 KCl_____Sylvite 0.000000000000000E+00
104 0.000000000000000E+00 K2Ca(SO4)2.H2O_____Syngenite 0.000000000000000E+00
105 0.000000000000000E+00 Mg2CaCl6.12H2O_____Tachyhydrite 0.000000000000000E+00
106 0.000000000000000E+00 Na2SO4_____Thenardite 0.000000000000000E+00
107 0.000000000000000E+00 Na2CO3.H2O_____Thermonatrite 0.000000000000000E+00
108 0.000000000000000E+00 Na3H(CO3)2.2H2O_____Trona 0.000000000000000E+00
109 0.000000000000000E+00 Na2B4O7.10H2O_____Borax 0.000000000000000E+00
110 0.000000000000000E+00 B(OH)3_____Borix_Acid_Solid 0.000000000000000E+00
111 0.000000000000000E+00 KB5O8.4H2O____K-Pentaborate_(30_C) 0.000000000000000E+00
112 0.000000000000000E+00 K2B4O7.4H2O___K-Tetraborate_(30_C) 0.000000000000000E+00
113 0.000000000000000E+00 NaBO2.4H2O_____Sodium_Metaborate 0.000000000000000E+00
114 0.000000000000000E+00 NaB5O8.5H2O_____Sodium_Pentaborate 0.000000000000000E+00
```

```
115  0.000000000000000E+00 NaBO2.NaCl.2H2O___Teepleite_(20_C) 0.000000000000000E+00
```

Appendix Q: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

See Table 17 for explanation of this listing.

```
 1 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.6imolal NaCl   FMT V2.3
 2   DATABASE:  NEA84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (HR94);
 3   95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RF794,RRF794)
 4
 5 Titrant Volumes per Grid Block, in milliliters
 6     1              0.000000 mL
 7     2              0.100000 mL
 8     3              0.142510 mL
 9     4              0.203092 mL
10     5              0.289427 mL
11     6              0.412463 mL
12     7              0.587802 mL
13     8              0.837678 mL
14     9              1.193777 mL
15    10              1.701254 mL
16    11              2.424462 mL
17    12              3.455107 mL
18    13              4.923883 mL
19    14              7.017038 mL
20    15             10.000000 mL
21
22
23 Titration Results, molal
24
25
26    0)  H2O          Na+          K+           Ca++         Mg++         MgOH+        H+           Cl-          SO4=
27    1)  1.92928E+01  5.61057E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.21872E-06  5.61096E+00  0.00000E+00
28    2)  1.92978E+01  5.61014E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.77346E-07  5.60993E+00  0.00000E+00
29    3)  1.92999E+01  5.61003E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  2.58813E-07  5.60950E+00  0.00000E+00
30    4)  1.93029E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.91065E-09  5.60889E+00  0.00000E+00
31    5)  1.93072E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.42512E-10  5.60800E+00  0.00000E+00
32    6)  1.93133E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.52979E-10  5.60671E+00  0.00000E+00
33    7)  1.93221E+01  5.61001E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  8.66954E-11  5.60491E+00  0.00000E+00
34    8)  1.93346E+01  5.61001E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.44489E-11  5.60233E+00  0.00000E+00
35    9)  1.93524E+01  5.61002E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.62550E-11  5.59866E+00  0.00000E+00
36   10)  1.93778E+01  5.61003E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  2.51081E-11  5.59343E+00  0.00000E+00
37   11)  1.94140E+01  5.61004E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.79163E-11  5.58601E+00  0.00000E+00
38   12)  1.94655E+01  5.61007E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.31074E-11  5.57548E+00  0.00000E+00
39   13)  1.95390E+01  5.61012E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.80463E-12  5.56057E+00  0.00000E+00
40   14)  1.96437E+01  5.61021E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  7.48733E-12  5.53952E+00  0.00000E+00
41   15)  1.97930E+01  5.61035E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.83272E-12  5.50989E+00  0.00000E+00
42
43    0)  HSO4-        OH-          HCO3-        CO3=         CO2(aq)      CaCO3(aq)    MgCO3(aq)    B(OH)3(aq)   B(OH)4-
44    1)  0.00000E+00  3.01685E-09  2.26571E-04  3.09384E-08  1.86103E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
45    2)  0.00000E+00  6.37029E-09  3.82212E-04  1.10196E-07  3.08476E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
46    3)  0.00000E+00  1.42123E-08  5.79856E-04  3.72979E-07  2.09763E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
47    4)  0.00000E+00  1.26397E-06  9.92660E-04  5.67888E-05  4.03745E-06  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
48    5)  0.00000E+00  1.07447E-05  1.00903E-03  4.90717E-04  4.82702E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
49    6)  0.00000E+00  2.40684E-05  1.02256E-03  1.11398E-03  2.18328E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
50    7)  0.00000E+00  4.34988E-05  1.04073E-03  2.00201E-03  1.25799E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
51    8)  0.00000E+00  6.77337E-05  1.06541E-03  3.26656E-03  8.07635E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
52    9)  0.00000E+00  1.01865E-04  1.09867E-03  5.06627E-03  5.53405E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
53   10)  0.00000E+00  1.47379E-04  1.14291E-03  7.62562E-03  3.97510E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
54   11)  0.00000E+00  2.07123E-04  1.20082E-03  1.12609E-02  2.96765E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
55   12)  0.00000E+00  2.84255E-04  1.27533E-03  1.64154E-02  2.29199E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
56   13)  0.00000E+00  3.82200E-04  1.36956E-03  2.37058E-02  1.82542E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
57   14)  0.00000E+00  5.04619E-04  1.48672E-03  3.39812E-02  1.49486E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
58   15)  0.00000E+00  6.55397E-04  1.63010E-03  4.83971E-02  1.25492E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
59
60    0)  B3O3(OH)4-   B4O5(OH)4=   CaB(OH)4+   MgB(OH)4+   Br-          ClO4-        NaOH(aq)     HCl(aq)      HClO4(aq)
61    1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
62    2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
63    3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
64    4)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
65    5)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
66    6)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
67    7)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
68    8)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
69    9)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
70   10)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
71   11)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
72   12)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
73   13)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
74   14)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
75   15)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
76
77    0)  PoSion.....  NegIon.....  PosIon(OH)(aq  NNegIon(aq)..  Tracer(aq)...  H3PO4(aq)    H2PO4-       HPO4=        PO4=-
78    1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
79    2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
80    3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
81    4)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
82    5)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
83    6)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
84    7)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
85    8)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
86    9)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
87   10)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
88   11)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
89   12)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
90   13)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
91   14)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
92   15)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
93
94    0)  NpO2+        NpO2OH(aq)   NpO2(OH)2-   NpO2CO3-     NpO2(CO3)2=- NpO2(CO3)3==- Am+++        AmCO3+       Am(CO3)2-
95    1)  6.12705E-04  7.72186E-10  2.04381E-16  1.33526E-07  1.98384E-11  1.25197E-16  0.00000E+00  0.00000E+00  0.00000E+00
96    2)  1.72085E-04  4.57851E-10  2.55903E-16  1.33573E-07  7.06677E-11  1.58546E-15  0.00000E+00  0.00000E+00  0.00000E+00
97    3)  5.08519E-05  3.01026E-10  3.76383E-16  1.33591E-07  2.39201E-10  1.81540E-14  0.00000E+00  0.00000E+00  0.00000E+00
98    4)  1.34101E-07  1.76139E-10  1.95583E-16  1.33613E-07  3.64205E-08  4.20660E-10  0.00000E+00  0.00000E+00  0.00000E+00
99    5)  1.86807E-08  1.73507E-10  1.63614E-13  1.33630E-07  3.14571E-07  3.13656E-08  0.00000E+00  0.00000E+00  0.00000E+00
100   6)  1.70494E-08  1.71249E-10  3.61806E-13  1.33654E-07  7.13649E-07  1.61312E-07  0.00000E+00  0.00000E+00  0.00000E+00
101   7)  9.49490E-09  1.68316E-10  6.28105E-13  1.33688E-07  1.28137E-06  5.19502E-07  0.00000E+00  0.00000E+00  0.00000E+00
102   8)  5.82643E-09  1.64493E-10  9.78743E-13  1.33737E-07  2.08796E-06  1.37733E-06  0.00000E+00  0.00000E+00  0.00000E+00
103   9)  3.76324E-09  1.59617E-10  1.42919E-12  1.33806E-07  3.23222E-06  3.29354E-06  0.00000E+00  0.00000E+00  0.00000E+00
104  10)  2.50641E-09  1.53503E-10  1.99133E-12  1.33905E-07  4.85191E-06  7.39875E-06  0.00000E+00  0.00000E+00  0.00000E+00
105  11)  1.70329E-09  1.46376E-10  2.67040E-12  1.34044E-07  7.13717E-06  1.59398E-05  0.00000E+00  0.00000E+00  0.00000E+00
106  12)  1.17412E-09  1.38078E-10  3.46327E-12  1.34242E-07  1.03461E-05  3.32873E-05  0.00000E+00  0.00000E+00  0.00000E+00
107  13)  8.18986E-10  1.28920E-10  4.35852E-12  1.34522E-07  1.48219E-05  6.77047E-05  0.00000E+00  0.00000E+00  0.00000E+00
108  14)  5.77122E-10  1.19205E-10  5.33952E-12  1.34916E-07  2.10028E-05  1.34208E-04  0.00000E+00  0.00000E+00  0.00000E+00
109  15)  4.11022E-10  1.09291E-10  6.38945E-12  1.35468E-07  2.94209E-05  2.58546E-04  0.00000E+00  0.00000E+00  0.00000E+00
110
111   0)  Am(CO3)3=-   Am(OH)2+    Am(OH)3(aq)  Th++++       UO2++        NpO2OH(aged)_ NpO2OH(amor)_ NaNpO2CO3(s)_ Na3NpO2(CO3)2
112   1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99932E+00  0.00000E+00
113   2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99718E+00  0.00000E+00
114   3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99612E+00  0.00000E+00
```

Appendix Q: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

115	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99673E+00	0.00000E+00
116	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99250E+00	0.00000E+00
117	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98931E+00	0.00000E+00
118	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98478E+00	0.00000E+00
119	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97832E+00	0.00000E+00
120	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96914E+00	0.00000E+00
121	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.95607E+00	0.00000E+00
122	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.93751E+00	0.00000E+00
123	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.91117E+00	0.00000E+00
124	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.87386E+00	0.00000E+00
125	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.82115E+00	0.00000E+00
126	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.74696E+00	0.00000E+00
127										
128	0)	AmOHCO3(c)___	Am(OH)3(a)___	NaAm(CO3)2.6H	AmPO4(c)_____	CaSO4_____	NaK3(SO4)2__A	CaCl2.6H2O__	CaCO3_____	K2SO4_____
129	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
130	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
131	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
132	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
133	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
134	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
135	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
136	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
137	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
138	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
139	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
140	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
141	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
142	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
143	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
144										
145	0)	MgCl2.6H2O___	Na2Mg(SO4)2.4	Mg(OH)2_____	Na6CO3(SO4)2_	CaCO3_____	CaCl2.4H2O__	Ca4Cl2(OH)6.1	Ca2Cl2(OH)2.H	KMgCl3.6H2O_
146	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
147	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
148	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
149	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
150	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
151	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
152	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
153	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
154	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
155	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
156	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
157	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
158	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
159	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
160	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
161										
162	0)	MgSO4.7H2O___	CaNa2(CO3)2.5	Na2Ca(SO4)2__	CaSO4.2H2O___	NaCl_____	MgSO4.6H2O__	KMgClSO4.3H2O	KHCO3_____	MgSO4.H2O____
163	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
164	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
165	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
166	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
167	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
168	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
169	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
170	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
171	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
172	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
173	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
174	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
175	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
176	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
177	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
178										
179	0)	K2Mg(SO4)2.4H	Na4Ca(SO4)3.2	MgCO3_____	Mg2Cl(OH)3.4H	KNSO4_____	Na2SO4.10H2O_	K8N6(SO4)7___	NaHCO3_____	Na2CO3.10H2O_
180	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
181	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
182	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
183	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
184	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
185	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
186	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
187	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
188	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
189	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
190	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
191	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
192	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
193	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
194	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
195										
196	0)	MgCO3.3H2O___	K2Mg(SO4)2.6H	Na2Ca(CO3)2.2	K2MgCa2(SO4)4	Ca(OH)2_____	K2CO3.3/2H2O_	K8N4(CO3)6.3H	KNaCO3.6H2O__	K2NaH(CO3)2.2
197	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
198	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
199	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
200	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
201	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
202	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
203	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
204	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
205	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
206	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
207	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
208	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
209	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
210	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
211	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
212										
213	0)	K3H(SO4)2__Sa	Na3H(SO4)2___	Na2CO3.7H2O__	KCl_____	K2Ca(SO4)2.H2	Mg2CaCl6.12H2	Na2SO4_____	Na2CO3.H2O___	Na3H(CO3)2.2H
214	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
215	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
216	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
217	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
218	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
219	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
220	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
221	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
222	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
223	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
224	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
225	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
226	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
227	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
228	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
229										
230	0)	Na2B4O7.10H2O	B(OH)3_____	KB5O8.4H2O___	K2B4O7.4H2O__	NaBO2.4H2O___	NaB5O8.5H2O__	NaBO2.NaCl.2H		
231	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
232	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
233	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
234	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
235	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
236	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
237	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
238	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		

Appendix Q: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

```
239   9)  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
240  10)  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
241  11)  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
242  12)  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
243  13)  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
244  14)  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
245  15)  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
246
247   0)  IonicStrength TitrVol.ml              pH          pmH
248   1)  5.61119E+00   0.0000000000E+00        5.320       5.914
249   2)  5.61031E+00   0.100000000            5.645       6.239
250   3)  5.61008E+00   0.142510267            5.994       6.587
251   4)  5.61006E+00   0.203091762            7.943       8.536
252   5)  5.61049E+00   0.289426612            8.872       9.465
253   6)  5.61112E+00   0.412462638            9.222       9.815
254   7)  5.61202E+00   0.587801607            9.469       10.06
255   8)  5.61330E+00   0.837677640            9.672       10.26
256   9)  5.61513E+00    1.19377664            9.849       10.44
257  10)  5.61774E+00    1.70125428            10.01       10.60
258  11)  5.62149E+00    2.42446202            10.16       10.75
259  12)  5.62685E+00    3.45510729            10.30       10.88
260  13)  5.63455E+00    4.92388263            10.42       11.01
261  14)  5.64559E+00    7.01703829            10.55       11.13
262  15)  5.66143E+00    10.0000000            10.66       11.23
```

Appendix R: Sample Output File "Np_NaCl_BM_LIN.TITRATE"

```
1 Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.3
2  DATABASE:  NEMB4/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
3  95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,F91,RSFR92,RSF94,RAFF94)
4
5  Titrant Volumes per Grid Block, in millilliters
6     1              0.000000 mL
7     2              0.100000 mL
8     3              0.200000 mL
9     4              0.300000 mL
10    5              0.400000 mL
11    6              0.500000 mL
12    7              0.600000 mL
13    8              0.700000 mL
14    9              0.800000 mL
15   10              0.900000 mL
16   11              1.000000 mL
17   12              1.100000 mL
18   13              1.200000 mL
19   14              1.300000 mL
20   15              1.400000 mL
21
22
23 Titration Results, molal
24
25
```

		H2O	Na+	K+	Ca++	Mg++	MgOH+	H+	Cl-	SO4=
26	0)	1.92928E+01	5.61057E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.21872E-06	5.61096E+00	0.00000E+00
27	1)	1.92978E+01	5.61014E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.77346E-07	5.60993E+00	0.00000E+00
28	2)	1.93027E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.87609E-09	5.60892E+00	0.00000E+00
29	3)	1.93077E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.09202E-10	5.60789E+00	0.00000E+00
30	4)	1.93127E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.61951E-10	5.60685E+00	0.00000E+00
31	5)	1.93177E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.10445E-10	5.60582E+00	0.00000E+00
32	6)	1.93227E+01	5.61001E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.42049E-11	5.60479E+00	0.00000E+00
33	7)	1.93277E+01	5.61001E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	6.82959E-11	5.60375E+00	0.00000E+00
34	8)	1.93327E+01	5.61001E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.76161E-11	5.60272E+00	0.00000E+00
35	9)	1.93377E+01	5.61001E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.99485E-11	5.60169E+00	0.00000E+00
36	10)	1.93427E+01	5.61001E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.41741E-11	5.60066E+00	0.00000E+00
37	11)	1.93477E+01	5.61002E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.96673E-11	5.59962E+00	0.00000E+00
38	12)	1.93527E+01	5.61002E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.60509E-11	5.59859E+00	0.00000E+00
39	13)	1.93577E+01	5.61002E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.30838E-11	5.59756E+00	0.00000E+00
40	14)	1.93627E+01	5.61002E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.06048E-11	5.59653E+00	0.00000E+00
41	15)									

		HSO4-	OH-	HCO3-	CO3=	CO2(aq)	CaCO3(aq)	MgCO3(aq)	B(OH)3(aq)	B(OH)4-
42										
43	0)	0.00000E+00	3.01685E-09	2.26571E-04	3.09384E-08	3.86103E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
44	1)	0.00000E+00	6.37029E-09	3.82212E-04	1.10196E-07	3.08476E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
45	2)	0.00000E+00	9.49137E-07	9.89705E-04	4.25167E-05	5.36072E-06	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
46	3)	0.00000E+00	1.19027E-05	1.01025E-03	5.44263E-04	4.36260E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
47	4)	0.00000E+00	2.27338E-05	1.02124E-03	1.05085E-03	2.30850E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
48	5)	0.00000E+00	3.33488E-05	1.03174E-03	1.55739E-03	1.58957E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
49	6)	0.00000E+00	4.37579E-05	1.04196E-03	2.06377E-03	1.22321E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
50	7)	0.00000E+00	5.39719E-05	1.05196E-03	2.56997E-03	1.00104E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
51	8)	0.00000E+00	6.40010E-05	1.06176E-03	3.07597E-03	8.51877E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
52	9)	0.00000E+00	7.38545E-05	1.07138E-03	3.58175E-03	7.44762E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
53	10)	0.00000E+00	8.35411E-05	1.08082E-03	4.08730E-03	6.64082E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
54	11)	0.00000E+00	9.30687E-05	1.09010E-03	4.59262E-03	6.01101E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
55	12)	0.00000E+00	1.02445E-04	1.09923E-03	5.09770E-03	5.50552E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
56	13)	0.00000E+00	1.11676E-04	1.10821E-03	5.60253E-03	5.09071E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
57	14)	0.00000E+00	1.20768E-04	1.11706E-03	6.10711E-03	4.74407E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
58	15)									

		B3O3(OH)4-	B4O5(OH)4=	CaB(OH)4+	MgB(OH)4+	Br-	ClO4-	NaOH(aq)	HCl(aq)	HClO4(aq)
59										
60	0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
61	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
62	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
63	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
64	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
65	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
66	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
67	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
68	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
69	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
70	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
71	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
72	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
73	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
74	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
75	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
76										

		PosIon.....	NegIon.....	PosIon(OH)(aq	NNegIon(aq)..	Tracer(aq)...	H3PO4(aq)	H2PO4-	HPO4=	PO4=-
77	0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
78	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
79	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
80	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
81	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
82	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
83	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
84	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
85	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
86	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
87	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
88	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
89	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
90	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
91	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
92	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
93										

		NpO2+	NpO2OH(aq)	NpO2(OH)2-	NpO2CO3-	NpO2(CO3)2=-	NpO2(CO3)3===	Am+++	AmCO3+	Am(CO3)2-
94	0)	6.12705E-04	7.72186E-10	2.04381E-16	1.33526E-07	1.98384E-11	1.25197E-16	0.00000E+00	0.00000E+00	0.00000E+00
95	1)	1.72085E-04	4.57851E-10	2.55903E-16	1.33573E-07	7.06677E-11	1.58546E-15	0.00000E+00	0.00000E+00	0.00000E+00
96	2)	4.46247E-07	1.76865E-10	1.47303E-14	1.33612E-07	2.72677E-08	2.35800E-10	0.00000E+00	0.00000E+00	0.00000E+00
97	3)	3.46770E-08	1.73100E-10	1.61034E-13	1.33622E-07	3.48878E-07	3.85776E-08	0.00000E+00	0.00000E+00	0.00000E+00
98	4)	1.80727E-08	1.71468E-10	3.42173E-13	1.33651E-07	6.72247E-07	1.43575E-07	0.00000E+00	0.00000E+00	0.00000E+00
99	5)	1.22005E-08	1.69754E-10	4.97012E-13	1.33671E-07	9.97249E-07	3.14830E-07	0.00000E+00	0.00000E+00	0.00000E+00
100	6)	9.21138E-09	1.68120E-10	6.45975E-13	1.33690E-07	1.32081E-06	5.51937E-07	0.00000E+00	0.00000E+00	0.00000E+00
101	7)	7.40067E-09	1.66553E-10	7.89467E-13	1.33710E-07	1.64391E-06	8.54484E-07	0.00000E+00	0.00000E+00	0.00000E+00
102	8)	6.18630E-09	1.65046E-10	9.27855E-13	1.33729E-07	1.96653E-06	1.22205E-06	0.00000E+00	0.00000E+00	0.00000E+00
103	9)	5.31533E-09	1.63595E-10	1.06147E-12	1.33749E-07	2.28868E-06	1.65423E-06	0.00000E+00	0.00000E+00	0.00000E+00
104	10)	4.66017E-09	1.62195E-10	1.19063E-12	1.33768E-07	2.61033E-06	2.15059E-06	0.00000E+00	0.00000E+00	0.00000E+00
105	11)	4.14945E-09	1.60844E-10	1.31559E-12	1.33788E-07	2.93150E-06	2.71072E-06	0.00000E+00	0.00000E+00	0.00000E+00
106	12)	3.74015E-09	1.59537E-10	1.43661E-12	1.33807E-07	3.25216E-06	3.33418E-06	0.00000E+00	0.00000E+00	0.00000E+00
107	13)	3.40480E-09	1.58274E-10	1.55392E-12	1.33827E-07	3.57233E-06	4.02056E-06	0.00000E+00	0.00000E+00	0.00000E+00
108	14)	3.12502E-09	1.57050E-10	1.66773E-12	1.33846E-07	3.89199E-06	4.76942E-06	0.00000E+00	0.00000E+00	0.00000E+00
109	15)									
110										

		Am(CO3)3=-	Am(OH)2+	Am(OH)3(aq)	Th++++	UO2++	NpO2OH(aqwd)	NpO2OH(amor)	NaNpO2CO3(s)	Na3NpO2(CO3)2
111	0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99832E+00	0.00000E+00
112	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99718E+00	0.00000E+00
113	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99481E+00	0.00000E+00
114	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99232E+00	0.00000E+00
115	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98964E+00	0.00000E+00
116	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98705E+00	0.00000E+00
117	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98446E+00	0.00000E+00
118	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98188E+00	0.00000E+00
119	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97930E+00	0.00000E+00
120	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		

Appendix R: Sample Output File "Np_NaCl_BM_LIN.TITRATE"

10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97672E+00	0.00000E+00		
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97413E+00	0.00000E+00		
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97156E+00	0.00000E+00		
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96898E+00	0.00000E+00		
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96640E+00	0.00000E+00		
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96382E+00	0.00000E+00		

	AmOHCO3(c)___	Am(OH)3(s)___	NaAm(CO3)2.6H	AmPO4(c)_____	CaSO4_____	NaK3(SO4)2__A	CaCl2.6H2O___	CaCO3_____	K2SO4_____
0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	MgCl2.6H2O___	Na2Mg(SO4)2.4	Mg(OH)2_____	Na6CO3(SO4)2_	CaCO3_____	CaCl2.4H2O___	Ca4Cl2(OH)6.1	Ca2Cl2(OH)2.H	KMgCl3.6H2O__
0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	MgSO4.7H2O___	CaNa2(CO3)2.5	Na2Ca(SO4)2__	CaSO4.2H2O___	NaCl_____	MgSO4.6H2O___	KMgCl6O4.3H2O	KHCO3_____	MgSO4.H2O____
0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	K2Mg(SO4)2.4H	Na4Ca(SO4)3.2	MgCO3_____	Mg2Cl(OH)3.4H	KHSO4_____	Na2SO4.10H2O_	K8H6(SO4)7___	NaHCO3_____	Na2CO3.10H2O_
0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	MgCO3.3H2O___	K2Mg(SO4)2.6H	Na2Ca(CO3)2.2	K2NgCa2(SO4)4	Ca(OH)2_____	K2CO3.3/2H2O_	K8H4(CO3)6.3H	KNaCO3.6H2O__	K2NaH(CO3)2.2
0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	K3H(SO4)2__Se	Na3H(SO4)2___	Na2CO3.7H2O__	KCl_____	K2Ca(SO4)2.H2	Mg2CaCl6.12H2	Na2SO4_____	Na2CO3.H2O___	Na3H(CO3)2.2H
0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	Na2B4O7.10H2O	B(OH)3_____	KB5O8.4H2O___	K2B4O7.4H2O__	NaBO2.4H2O___	Na2B5O8.5H2O__	NaBO2.NaCl.2H
0)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

Appendix R: Sample Output File "Np_NaCl_BM_LIN.TITRATE"

245	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
246								
247	0)	IonicStrength	TitrVol,ml		pH	pmH		
248	1)	5.61119E+00	0.000000000E+00		5.320	5.914		
249	2)	5.61031E+00	0.100000000		5.665	6.239		
250	3)	5.61004E+00	0.200000000		7.818	8.412		
251	4)	5.61055E+00	0.300000000		8.917	9.510		
252	5)	5.61106E+00	0.400000000		9.198	9.791		
253	6)	5.61157E+00	0.500000000		9.364	9.957		
254	7)	5.61208E+00	0.600000000		9.482	10.07		
255	8)	5.61259E+00	0.700000000		9.573	10.17		
256	9)	5.61310E+00	0.800000000		9.647	10.24		
257	10)	5.61362E+00	0.900000000		9.710	10.30		
258	11)	5.61413E+00	1.00000000		9.763	10.35		
259	12)	5.61464E+00	1.10000000		9.810	10.40		
260	13)	5.61516E+00	1.20000000		9.852	10.44		
261	14)	5.61567E+00	1.30000000		9.889	10.48		
262	15)	5.61619E+00	1.40000000		9.923	10.51		

Appendix S: Sample Output File "Np_NaCl_BM.TITRATE"

```
Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.3
 DATABASE:  JOM94/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

Titrant Volumes per Grid Block, in milliliters
     1            0.000000 mL
     2            0.100000 mL
     3            0.142510 mL
     4            0.160000 mL
     5            0.180000 mL
     6            0.203090 mL
     7            0.220900 mL
     8            0.240000 mL
     9            0.260000 mL
    10            0.289430 mL
    11            0.412460 mL
    12            0.587800 mL
    13            1.193800 mL
    14            3.455100 mL
    15           10.000000 mL


Titration Results, molal

    0)  H2O          Na+          K+           Ca++         Mg++         MgOH+        H+           Cl-          SO4=
    1)  1.92928E+01  5.61057E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.21672E-06  5.61096E+00  0.00000E+00
    2)  1.92978E+01  5.61014E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.77346E-07  5.60993E+00  0.00000E+00
    3)  1.92999E+01  5.61003E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  2.58815E-07  5.60950E+00  0.00000E+00
    4)  1.93007E+01  5.61001E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.48181E-07  5.60933E+00  0.00000E+00
    5)  1.93017E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.09374E-08  5.60913E+00  0.00000E+00
    6)  1.93029E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  2.91107E-09  5.60889E+00  0.00000E+00
    7)  1.93037E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.18855E-09  5.60872E+00  0.00000E+00
    8)  1.93047E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  6.93877E-10  5.60851E+00  0.00000E+00
    9)  1.93057E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  4.89995E-10  5.60830E+00  0.00000E+00
   10)  1.93072E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.42501E-10  5.60800E+00  0.00000E+00
   11)  1.93133E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.52981E-10  5.60673E+00  0.00000E+00
   12)  1.93221E+01  5.61001E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  8.66958E-11  5.60491E+00  0.00000E+00
   13)  1.93524E+01  5.61002E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.62542E-11  5.59866E+00  0.00000E+00
   14)  1.94655E+01  5.61007E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.31074E-11  5.57548E+00  0.00000E+00
   15)  1.97930E+01  5.61035E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.83272E-12  5.50989E+00  0.00000E+00

    0)  HSO4-        OH-          HCO3-        CO3=         CO2(aq)      CaCO3(aq)    MgCO3(aq)    B(OH)3(aq)   B(OH)4-
    1)  0.00000E+00  3.01685E-09  2.26571E-04  3.09384E-08  3.86103E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    2)  0.00000E+00  6.37029E-09  3.82212E-04  1.10196E-07  3.08476E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    3)  0.00000E+00  1.42122E-08  5.79854E-04  3.72976E-07  2.09764E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    4)  0.00000E+00  2.47909E-08  7.06447E-04  7.92644E-07  1.46506E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    5)  0.00000E+00  7.22202E-08  8.74979E-04  2.86004E-06  6.22872E-05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    6)  0.00000E+00  1.26379E-06  9.92658E-04  5.67805E-05  4.03803E-06  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    7)  0.00000E+00  1.09556E-06  9.99205E-04  1.39997E-04  1.65938E-06  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    8)  0.00000E+00  5.30281E-06  1.00274E-03  2.40670E-04  9.72059E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    9)  0.00000E+00  7.50984E-06  1.00546E-03  3.41763E-04  6.88224E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   10)  0.00000E+00  1.07451E-05  1.00903E-03  4.90734E-04  4.82685E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   11)  0.00000E+00  2.40681E-05  1.02256E-03  1.11397E-03  2.18331E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   12)  0.00000E+00  4.24987E-05  1.04073E-03  2.00200E-03  1.25799E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   13)  0.00000E+00  1.01868E-04  1.09867E-03  5.06639E-03  5.53395E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   14)  0.00000E+00  2.84255E-04  1.27533E-03  1.64154E-02  2.29199E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   15)  0.00000E+00  6.55397E-04  1.63010E-03  4.83971E-02  1.25492E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

    0)  B3O3(OH)4-   B4O5(OH)4=  CaB(OH)4+  MgB(OH)4+  Br-          ClO4-        NaOH(aq).....  HCl(aq).....  HClO4(aq).....
    1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    4)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    5)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    6)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    7)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    8)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    9)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   10)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   11)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   12)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   13)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   14)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   15)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

    0)  PosIon.....  NegIon.....  PosIon(ON)(aq  NNegIon(aq)..  Tracer(aq)...  H3PO4(aq)    H2PO4-       HPO4=        PO4=-
    1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    4)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    5)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    6)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    7)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    8)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
    9)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   10)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   11)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   12)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   13)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   14)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
   15)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

    0)  NpO2+        NpO2OH(aq)   NpO2(OH)2-   NpO2CO3-     NpO2(CO3)2=- NpO2(CO3)3=-- Am+++        AmCO3+       Am(CO3)2-
    1)  6.12705E-04  7.72186E-10  2.04381E-16  1.33526E-07  1.98384E-11  1.25197E-16  0.00000E+00  0.00000E+00  0.00000E+00
    2)  1.72085E-04  4.57851E-10  2.55903E-16  1.33573E-07  7.06677E-11  1.58546E-15  0.00000E+00  0.00000E+00  0.00000E+00
    3)  5.08524E-05  3.01827E-10  3.76382E-16  1.33591E-07  2.39199E-10  1.81536E-14  0.00000E+00  0.00000E+00  0.00000E+00
    4)  2.39107E-05  2.47753E-10  5.38926E-16  1.33598E-07  5.08355E-10  8.19789E-14  0.00000E+00  0.00000E+00  0.00000E+00
    5)  6.63303E-06  2.00045E-10  1.26769E-15  1.33606E-07  1.83431E-09  1.06720E-12  0.00000E+00  0.00000E+00  0.00000E+00
    6)  3.14150E-07  1.76340E-10  1.95555E-14  1.33613E-07  1.64151E-08  4.20517E-10  0.00000E+00  0.00000E+00  0.00000E+00
    7)  1.35537E-07  1.75190E-10  4.75887E-14  1.33616E-07  8.97771E-08  2.55580E-09  0.00000E+00  0.00000E+00  0.00000E+00
    8)  7.88495E-08  1.74579E-10  8.12402E-14  1.33620E-07  1.54320E-07  7.55070E-09  0.00000E+00  0.00000E+00  0.00000E+00
    9)  5.55313E-08  1.74113E-10  1.14749E-13  1.33624E-07  2.19119E-07  1.52213E-08  0.00000E+00  0.00000E+00  0.00000E+00
   10)  3.86794E-08  1.73507E-10  1.63619E-13  1.33630E-07  3.14582E-07  3.13678E-08  0.00000E+00  0.00000E+00  0.00000E+00
   11)  1.70496E-08  1.71249E-10  3.61801E-13  1.33654E-07  7.13640E-07  1.61208E-07  0.00000E+00  0.00000E+00  0.00000E+00
   12)  9.49502E-09  1.68316E-10  6.28103E-13  1.33688E-07  1.28136E-06  5.19497E-07  0.00000E+00  0.00000E+00  0.00000E+00
   13)  3.76315E-09  1.59617E-10  1.42922E-12  1.33806E-07  3.23230E-06  3.39369E-06  0.00000E+00  0.00000E+00  0.00000E+00
   14)  1.17432E-09  1.38078E-10  3.46327E-12  1.34242E-07  1.03462E-05  3.32671E-05  0.00000E+00  0.00000E+00  0.00000E+00
   15)  4.11022E-10  1.09291E-10  6.38945E-12  1.35468E-07  2.94209E-05  2.58546E-04  0.00000E+00  0.00000E+00  0.00000E+00

    0)  Am(CO3)3=-   Am(OH)2+    Am(OH)3(aq)  Th++++       UO2++        NpO2OH(aged)_ NpO2OH(amor)_ NaNpO2CO3(s)_ Na3NpO2(CO3)2
    1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99932E+00  0.00000E+00
    2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99718E+00  0.00000E+00
    3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99622E+00  0.00000E+00
    4)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99580E+00  0.00000E+00
    5)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99531E+00  0.00000E+00
    6)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99473E+00  0.00000E+00
    7)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99430E+00  0.00000E+00
    8)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99378E+00  0.00000E+00
    9)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99326E+00  0.00000E+00
```

Appendix S: Sample Output File "Np_NaCl_BM.TITRATE"

121	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99250E+00	0.00000E+00
122	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98931E+00	0.00000E+00
123	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98478E+00	0.00000E+00
124	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96914E+00	0.00000E+00
125	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.91117E+00	0.00000E+00
126	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.74696E+00	0.00000E+00
127										
128	0)	Am(OH)CO3(c)	Am(OH)3(s)	NaAm(CO3)2.6H	AmPO4(c)	CaSO4	NaK3(SO4)2:A	CaCl2.6H2O	CaCO3	K2SO4
129	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
130	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
131	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
132	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
133	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
134	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
135	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
136	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
137	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
138	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
139	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
140	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
141	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
142	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
143	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
144										
145	0)	MgCl2.6H2O	Na2Mg(SO4)2.4	Mg(OH)2	Na6CO3(SO4)2	CaCO3	CaCl2.4H2O	Ca4Cl2(OH)6.1	Ca2Cl2(OH)2.H	KMgCl3.6H2O
146	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
147	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
148	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
149	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
150	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
151	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
152	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
153	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
154	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
155	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
156	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
157	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
158	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
159	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
160	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
161										
162	0)	MgSO4.7H2O	CaNa2(CO3)2.5	Na2Ca(SO4)2	CaSO4.2H2O	NaCl	MgSO4.6H2O	KMgClSO4.3H2O	KHCO3	MgSO4.H2O
163	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
164	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
165	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
166	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
167	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
168	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
169	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
170	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
171	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
172	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
173	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
174	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
175	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
176	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
177	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
178										
179	0)	K2Mg(SO4)2.4H	Na4Ca(SO4)3.2	MgCO3	Mg2Cl(OH)3.4H	KHSO4	Na2SO4.10H2O	K8H6(SO4)7	NaHCO3	Na2CO3.10H2O
180	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
181	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
182	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
183	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
184	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
185	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
186	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
187	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
188	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
189	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
190	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
191	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
192	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
193	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
194	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
195										
196	0)	MgCO3.3H2O	K2Mg(SO4)2.6H	Na2Ca(CO3)2.2	K2MgCa2(SO4)4	Ca(OH)2	K2CO3.3/2H2O	K8H4(CO3)6.3H	KNaCO3.6H2O	K2NaH(CO3)3.2
197	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
198	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
199	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
200	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
201	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
202	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
203	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
204	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
205	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
206	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
207	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
208	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
209	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
210	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
211	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
212										
213	0)	K3H(SO4)2:Se	Na3H(SO4)2	Na2CO3.7H2O	KCl	K2Ca(SO4)2.H2	Mg2CaCl6.12H2	Na2SO4	Na2CO3.H2O	Na3H(CO3)2.2H
214	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
215	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
216	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
217	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
218	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
219	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
220	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
221	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
222	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
223	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
224	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
225	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
226	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
227	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
228	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
229										
230	0)	Na2B4O7.10H2O	B(OH)3	KB5O8.4H2O	K2B4O7.4H2O	NaBO2.4H2O	NaB5O8.5H2O	NaBO2.NaCl.2H		
231	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
232	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
233	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
234	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
235	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
236	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
237	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
238	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
239	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
240	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
241	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
242	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
243	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
244	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		

Appendix S: Sample Output File "Np_NaCl_BM.TITRATE"

```
 15)  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00

  0)  IonicStrength TitrVol,ml          pH           pmH
  1)  5.61119E+00   0.000000000E+00    5.320        5.914
  2)  5.61031E+00   0.100000000        5.645        6.239
  3)  5.61008E+00   0.142510000        5.994        6.587
  4)  5.61003E+00   0.160000000        6.235        6.829
  5)  5.61001E+00   0.180000000        6.700        7.293
  6)  5.61006E+00   0.203090000        7.943        8.536
  7)  5.61014E+00   0.220000000        8.332        8.925
  8)  5.61024E+00   0.240000000        8.565        9.159
  9)  5.61034E+00   0.260000000        8.717        9.310
 10)  5.61049E+00   0.289430000        8.872        9.465
 11)  5.61112E+00   0.412460000        9.222        9.815
 12)  5.61202E+00   0.587800000        9.469        10.06
 13)  5.61513E+00   1.19380000         9.849        10.44
 14)  5.62685E+00   3.45510000         10.30        10.88
 15)  5.66143E+00   10.0000000         10.66        11.23
```

Appendix T: Command File FMT_CUR.COM

```
$!    SET noverify
$!    SET verify
$!          FMT_CUR.COM assigns and fetches user-selected
$!          chemdat and rhomin data base file names,
$!          assign user-specified input/output file names,
$!          executes fmt-fmt in CMS 1997 nonPA (Performance
$!          Asssessment) production area
$!          Copied from FMT_FMTC.COM
$!
$!           Modifier: S. C. Babb
$!           Date:     03/31/97
$!           Reason:   query user on PRINT/NOPRINT chemdat db in OUT file
$!             set executable to fmt vs2.3
$!
$!           Modifier: S. C. Babb
$!           Date:     04/29/97
$!           Reason:   write input/output filenames and linker information
$!                     to log file
$!
$!*******************************************************************************
*
$!   INPUTS:
$!
$!      P1 - Substring chemdat file name search on valance states, dates,
$!        and/or fugacity
$!
$!      P2 - Substring rhomin file name search on valance states and/or dates
$!
$!      P3 - Input File Name (no extension)
$!
$!      P4 - Directory where Input Files located (optional)
$!
$!-------------------------------------------------------------------------------
-
$!
$! Turn on error handling; exit on any error.
$!
$    ON error then goto error_exit
$    mode = f$mode()
$!
$! Logic flow
$!
$!   Optional - Set P4 - this is the directory where input files are located,
$!   SCMS files are fetched to and output files are generated
$!
$   IF p4 .nes. ""
$    THEN
$     set default 'p4'
$    ENDIF
$!
$    GOSUB check_filename
$    GOSUB define_cms_library
$    GOSUB delete_files
$    GOSUB get_database_files
$    GOSUB define_inputs
$    GOSUB define_outputs
$    GOSUB start_log
$!    GOSUB start_mail
$    GOSUB run_fmt
$    GOSUB undefine_symbols
$    EXIT
```

```
$!-------------------------------------------------------------------------------
$CHECK_FILENAME:
$! Determine if any or all file names are passed as parameters. If not,
$! prompt for one if this is an interactive session;
$! otherwise flag an error and exit
$!
$!  Check for P1 - this is the CHEMDAT name field
$!
$  IF mode .eqs. "BATCH" .and. p1 .eqs. ""
$  THEN
$      WRITE sys$output -
      "Can not run in batch without a chemdat file name (P1). exiting."
$      GOTO error_exit
$  ENDIF
$!
$!
$  IF p1 .eqs. ""
$   THEN
$       INQUIRE chemdat_name  -
                  "Enter chemdat file name to search on"
$       IF chemdat_name .eqs. "" THEN goto error_exit
$  ELSE
$       chemdat_name = p1
$  ENDIF
$!
$!  Check for P2 - this is the RHOMIN name field
$!
$  IF mode .eqs. "BATCH" .and. p2 .eqs. ""
$  THEN
$      WRITE sys$output -
      "Can not run in batch without a rhomin file name (P2). exiting."
$      GOTO error_exit
$  ENDIF
$!
$!
$  IF p2 .eqs. ""
$   THEN
$       INQUIRE rhomin_name  -
                  "Enter rhomin file name to search on"
$       IF rhomin_name .eqs. "" THEN goto error_exit
$   ELSE
$       rhomin_name = p2
$   ENDIF
$!
$!  Check for P3 - this is the file name field
$!
$  IF mode .eqs. "BATCH" .and. p3 .eqs. ""
$  THEN
$      WRITE sys$output -
      "Can not run in batch without a file name (P3). exiting."
$      GOTO error_exit
$  ENDIF
$!
$!
$  IF p3 .eqs. ""
$   THEN
$       INQUIRE file_name  "Enter input file name (without .extension)"
$       IF file_name .eqs. "" THEN goto error_exit
$  ELSE
$       file_name = p3
$  ENDIF
$   RETURN
$!-------------------------------------------------------------------------------
```

```
$DEFINE_CMS_LIBRARY:
$! Define non-pa cms symbols and point to fmt library
$!
$!  set noverify
$  nonpa_cms_syms
$!
$! Set CMS library to FMT
$!
$    cms_library_name = "fmt"
$    lib'cms_library_name
$!  set verify
$!
$    RETURN
$!-------------------------------------------------------------------------
$DEFINE_INPUTS:
$! Define the input files needed.
$!
$    DEFINE input 'file_name'.in
$    DEFINE inguess 'file_name'.inguess
$!
$! Define a logical that points to the database files just fetched
$!
$    DEFINE chemdat 'chemdat_name'
$    DEFINE rhomin 'rhomin_name'
$!
$    RETURN
$!-------------------------------------------------------------------------
-
$DEFINE_OUTPUTS:
$! Define the output files needed.
$!
$    DEFINE output 'file_name'.out
$    DEFINE for088 'file_name'.for088
$    DEFINE titrate 'file_name'.titrate
$!
$    RETURN
$!-------------------------------------------------------------------------
-
$DELETE_FILES:
$!
$! Turn off warning messages for no files to delete
$!
$    SET noon
$    SET message/nofac/nosev/notext/noid
$! Delete all 'file_name'.moles files; do not accumulate them.
$!
$    DELETE  'file_name'.moles;*
$! Delete all fmt prefixed files of chemdat and rhomin files
$!
$    DELETE  fmt_*.chemdat;*
$    DELETE  fmt_*.rhomin;*
$    SET message/fac/sev/text/id
$    SET on
$!
$    RETURN
$!-------------------------------------------------------------------------
-
$ERROR_EXIT:
$! Exit routine when a severe error is encountered
$!
$    Write sys$output "Executing error exit, ''$status'."
$    EXIT
```

```
$!-------------------------------------------------------------------------------
-
$GET_DATABASE_FILES:
$!
$! If interactive, allow user to select/pick from a list of chemdat file names
$!
$  IF mode .nes. "BATCH"
$  THEN
$    cse "*''chemdat_name'*.chemdat"
$!
$    INQUIRE chemdat_name "Select CHEMDAT name from list above"
$  ENDIF
$!
$! Fetch chemdat from FMT CMS
$!
$!   set noverify
$    cfe 'chemdat_name'
$!   set verify
$!
$! If interactive allow user to select/pick from a list of rhomin file names
$!
$  IF mode .nes. "BATCH"
$  THEN
$    cse "*''rhomin_name'*.rhomin"
$!
$    INQUIRE rhomin_name "Select RHOMIN name from list above"
$  ENDIF
$!
$! Fetch chemdat from FMT CMS
$!   set noverify
$    cfe 'rhomin_name'
$!   set verify
$!
$    RETURN
$!-------------------------------------------------------------------------------
-
$RUN_FMT:
$!
$! Write the image information in the log file
$! Define the run symbols needed.
$   define /nolog exe_dir
wp$nonpa_prodroot:[fmt.exe]
$    fmt   :== "$exe_dir:fmt_pa97.exe"
$!
$! Run the utility that shows image information from the exe. (mandatory!)
$! This is part of the documentation required while doing a calculation.
$  @wp$ref:wp_get_image_id.com
exe_dir:fmt_pa97.exe
$!
$! Get user input for print/noprint of chemdat parameters in the out file
$! define/user sys$input sys$command
$    inquire answer "Enter ""Y"" or ""y"" to echo database in OUT file"
$!
$    if answer .eqs. "Y" then goto close_log_file
$    if answer .eqs. "y" then goto close_log_file
$    write sys$output "Pitzer Data Base NOT echoed in this Run"
$close_log_file:
$    deassign sys$output
$!
$! Write information to the user's screen
$! Run the utility that shows image information from the exe. (mandatory!)
$! This is part of the documentation required while doing a calculation.
```

```
$  @wp$ref:wp_get_image_id.com
exe_dir:fmt_pa97.exe
$!
$! Run the code
$  fmt 'answer'
$  RETURN
$!-------------------------------------------------------------------------
-
$START_LOG:
$!
$!
$  month   ==    f$cvtime("''f$time()'", "absolute", "month" )
$  day      ==   f$cvtime("''f$time()'", "comparison", "day" )
$  hour    ==    f$cvtime("''f$time()'", "absolute", "hour" )
$  min      ==  f$cvtime("''f$time()'", "absolute", "minute" )
$!
$  log_file_name :== "''file_name'_''month'''day'_''hour'''min'.log"
$!  mike williamson's log file definition:
$!   "sys$login:fmt_''file_name'_''month'''day'_''hour'''min'.log"
$!
$  DEFINE/proc sys$output 'log_file_name
$! Write the input file names
$      show logical input
$      show logical inguess
$! Write the data base file names
$      show logical chemdat
$      show logical rhomin
$! Write the output file names
$      show logical output
$      show logical for088
$      show logical titrate
$!
$  RETURN
$!-------------------------------------------------------------------------
$START_MAIL:
$! Open a file where we can write a message that can be sent to the
$! user upon completion.
$!
$  mail_error_flag = 0
$  mail_file_name :== "sys$Login:fmt_mail.msg"
$  mail_subject   :== "FMT ''file_name' run."
$  mail_list == f$getjpi( "", "username")
$!
$  OPEN/write mail_file 'mail_file_name
$!
$  RETURN

$!-------------------------------------------------------------------------
-
$TERMINATE:
$! If there was no previously flagged error or problem, search the log files
$! for any fatal, error, or warning messages.
$!
$! Deassign sys$output so the "log" file closes.
$   deassign sys$output
$!
$! Show the run output to the user
$   TYPE 'log_file_name
$!
$! Skip sending the mail message
$   goto end_terminate
$!
$! If there was not a previous error recorded, search the log file for
```

```
$! common error indicators.
$    search_status = 0
$    IF mail_error_flag .ne. 1
$    THEN
$!       Turn off informational messages from search command
$        SET message/nofac/nosev/notext/noid
$     SEARCH 'log_file_name "-F-","-E-","-W-" / match=or
$     search_status = $status
$!       Turn on messages
$        SET message/fac/sev/text/id
$    ENDIF
$!
$    IF search_status .eq. 1 .or. mail_error_flag .eq. 1
$    THEN
$     WRITE mail_file  "The run log contains an error or warning. "
$     WRITE mail_file  "Please examine ''log_file_name'."
$     mail_subject    == "''mail_subject' ERROR"
$    ELSE
$     WRITE mail_file  "The FMT run has completed."
$    ENDIF
$!
$    CLOSE/nolog mail_file
$    MAIL/subject="''mail_subject'" 'mail_file_name 'mail_list
$!
$END_TERMINATE:
$    EXIT
$!-------------------------------------------------------------------------------
$UNDEFINE_SYMBOLS:
$! Deassign input files
$!
$    DEASSIGN input
$    DEASSIGN inguess
$    DEASSIGN chemdat
$    DEASSIGN rhomin
$    DEASSIGN output
$    DEASSIGN for088
$    DEASSIGN titrate
$!
$    RETURN
$!-------------------------------------------------------------------------------
-
$! CMS REPLACEMENT HISTORY, Element FMT_FMTC.COM
$! *3     23-SEP-1996 09:09:31 SCBABB "ADD PARAMETER P4 FOR BATCH RUNS"
$! *2     21-DEC-1995 12:58:57 SCBABB "FMT EXECUTABLE NAME CHANGED"
$! *1     19-DEC-1995 12:26:54 SCBABB "USER COMMAND FILE FOR EXECUTING
FMT_FMT2P0 FROM CMS"
$! CMS REPLACEMENT HISTORY, Element FMT_FMTC.COM
```

Appendix U: Derivation of CO_2 Fugacity

The derivation of the expression for calculating for CO_2 (g) fugacity within FMT is given below.

The CO_2 equilibrium reaction can be written as:

$$CO_2(g) + H_2O \rightarrow 2H^+ + CO_3^{2-} \quad (1)$$

The equilibrium expression corresponding to this reaction is

$$K^{eq} = \frac{\left({}^{a}H^{+}\right)^2\left({}^{a}CO_3^{2-}\right)}{f_{CO_2(g)}{}^{a}H_2O} \quad (2)$$

Taking the $\log_{10}$ of this expression and rearranging terms yield

$$\log f_{co_2(g)} = 2\log a_{H^+} + \log a_{CO_3^{2-}} - \log a_{H_2O} - \log K^{eq} \quad (3)$$

or, since $pH \equiv -\log a_{H^+}$,

$$\log f_{co_2(g)} = -2pH + \log a_{CO_3^{2-}} - \log a_{H_2O} - \log K^{eq} \quad (4)$$

The equilibrium constant, K^{eq}, is related to the free energy change of reaction, ΔG°_{RXN}, by the expression

$$K^{eq} = \exp\left(\frac{-\Delta G^{\circ}_{RXN}}{RT}\right) \quad (5)$$

The ΔG°_{RXN} is related to the standard chemical potentials of the species shown in reaction equation 1 by the expression

$$\frac{\Delta G^{\circ}_{RXN}}{RT} = \frac{\mu^{\circ}_{H+}}{RT} + \frac{\mu^{\circ}_{CO_3^{2-}}}{RT} - \frac{\mu^{\circ}_{CO_2(g)}}{RT} - \frac{\mu^{\circ}_{H_2O}}{RT} \quad (6)$$

Substituting values for the standard chemical potentials, Equation 6 becomes

$$\frac{\Delta G^{\circ}_{RXN}}{RT} = 2(0) + (-212.944) - (-159.092) - (-95.6635) = 41.8115 \quad (7)$$

Therefore, $K^{eq} = 6.9422\times10^{-19}$, and $\log K^{eq} = -18.1585$.

The equation for the $\log_{10}$ of CO_2 fugacity can be simplified to

$$\log f_{co_2(g)} = -2pH + \log a_{CO_3^{2-}} - \log a_{H_2O} + 18.1585 \quad (8)$$

Appendix V: Memorandum on Current Release of Data Base

Sandia National Laboratories
Operated for the U.S. Department of Energy by
LOCKHEED MARTIN
Albuquerque, New Mexico 87185-1320

date: 23 August 1996

to: Robert C. Moore, Org. 6832, MS 1341

from: Craig F. Novak, Org. 6832, MS 1320

subject: Release of FMT Data Base File HMW_Am3Pu3Th4Np5_960823.CHEMDAT

The FMT data base files HMW_Am3Pu3Th4Np5_960823.CHEMDAT and HMW_Am3Pu3Th4Np5_960823.RHOMIN are available for use. These files contains the most complete set of thermodynamic data available for predicting dissolved actinide concentrations in concentrated electrolytes for the WIPP. The data base explicitly includes the actinides Am(III), Pu(III), Th(IV), and Np(V). Major interactions between these actinides and inorganic brine constituents, e.g., Na^+, K^+, Mg^{2+}, OH^-, Cl^-, CO_3^{2-}, and SO_4^{2-}, are included, but data and parameter values are not available or necessary for every combination of actinide and ligand. This release of the CHEMDAT and RHOMIN data base files completely replaces all previous versions.

Preliminary parameter values for major interactions between these actinides and the organic acid anions (OAAs) acetate, citrate, EDTA, lactate, and oxalate are included in the data base, as well as the dependence of actinide-OAA complexation on NaCl concentration. These values have not yet been finalized, and thus are not documented in this memorandum. The user of the CHEMDAT data base should critically assess the applicability and sources of the organic ligand parameters before making use of these values. Once documentation of the final values of the actinide-OAA parameters is available, these values will be incorporated into a new release of the CHEMDAT data base.

There has been a major reordering of chemical species within the CHEMDAT file accompanying this release. The INGUESS files prepared for use with previous releases of CHEMDAT cannot be used directly with this release. Because the element list is for the most part unchanged (the element entry for U(VI) was replaced with Pu(III)), lists of total element abundances can be used directly from older versions of CHEMDAT as long as U(VI) was not in the original problem. The incomplete nature of the U(VI) data base required its removal from CHEMDAT.

The data base contains preliminary values for U(IV) thermodynamic parameters. However, these are not discussed here because not all of the relevant chemical effects important to the WIPP system have been included. Despite being contained in this release, these values are not supported and should not be used for WIPP application.

This memorandum is intended to be a stand-alone document as much as possible, listing every parameter value that is included relevant to the actinides. Published sources are given wherever possible.

Data Sources, Inorganic, NonActinide Parameters

The CHEMDAT data base is an extension of the Harvie-Møller-Weare/Felmy-Weare (HMW/FW) (Harvie et al., 1984) parameterization of the Pitzer activity coefficient model for the brine-evaporite, or sea water, system. Harvie et al. (1984) parameterized the system Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O; Felmy and Weare (1986) extended this to include boron species. The HMW/FW data base serves as the primary source of thermodynamic parameters for the CHEMDAT data base. Parameters in these sources are not included in this memorandum. An auxiliary source for reference values is Pitzer (1991). Some parameters from this source are reproduced here.

Data Sources, Parameters for Actinide Interactions with Inorganic Ligands

The primary sources of thermodynamic parameter values for actinide interactions with inorganic ions are listed below. The listed references do not necessarily contain the original determination of the parameter values, but do list the parameters or sufficient information from which to calculate the parameters. The indicated references are sufficient for comparison and inspection of all of the parameter values given in the CHEMDAT file, although some unit conversion may be required.

Am(III)/Pu(III) Parameter Values

Dimensionless standard chemical potential (DSCP) values and ion interaction parameters for Am(III) and Pu(III) inorganic species are given in Tables 1 and 2, respectively. These models were developed from a combination of data from Am(III), Pu(III), and Nd(III). The Am(III) and Pu(III) models are identical in this release, although they may not be in future releases. The DSCPs are related by

$$\frac{\overset{\circ}{\mu}}{RT}(\text{Pu(III) Species}) = -\frac{\overset{\circ}{\mu}}{RT}(\text{Am(III) Species}) \; \nu\left(\frac{\overset{\circ}{\mu}}{RT}(Am^{3+}) - \frac{\overset{\circ}{\mu}}{RT}(Pu^{3+})\right) \quad (1)$$

or

$$\frac{\overset{\circ}{\mu}}{RT}(\text{Pu(III) Species}) = \frac{\overset{\circ}{\mu}}{RT}(\text{Am(III) Species}) + \nu\, 8.294 \quad (2)$$

where ν is the stoichiometric coefficient of Pu(III) and Am(III) in the species. The related equations between Am(III) and Nd(III) species are

$$\frac{\overset{\circ}{\mu}}{RT}(\text{Am(III) Species}) = \frac{\overset{\circ}{\mu}}{RT}(\text{Nd(III) Species}) - \nu\left(\frac{\overset{\circ}{\mu}}{RT}(Nd^{3+}) - \frac{\overset{\circ}{\mu}}{RT}(Am^{3+})\right) \quad (3)$$

or

$$\frac{\overset{\circ}{\mu}}{RT}(\text{Am(III) Species}) = \frac{\overset{\circ}{\mu}}{RT}(\text{Nd(III) Species}) + \nu\, 29.232 \quad (4)$$

where $\frac{\overset{\circ}{\mu}}{RT}(Nd^{3+}) = -270.926$ (Rao et al., 1996).

The binary interaction parameters values used for Am^{3+}-Cl^- require special attention. The values in the data base, as given in Table 2, are those used to develop all other +III actinide parameters except those in Fanghänel et al. (1995), who used the updated set 0.05856, 5.6, and –0.019 from Pitzer (1991). This introduces an inconsistency in the data base with respect to the trivalent actinide species and all parameters developed from these values. The only affected interpretation is that of data from Cl^- media where the free ion is the dominant form of the trivalent actinide, i.e., the determination of the DSCP for $Pu(OH)_3(s)$. The effect is small and appears to be of no significance for WIPP applications of this data base.

Th(IV) Parameter Values

Dimensionless standard chemical potential (DSCP) values and ion interaction parameters for Th(IV) inorganic species are given along with their sources in Tables 3 and 4, respectively.

Parameters for the Li^+ and NH_4^+ systems with Th^{4+} and SO_4^{2-}, not reproduced here, are given in Felmy and Rai (1992).

Np(V)/Pu(V)/Am(V) Parameter Values

Dimensionless standard chemical potential (DSCP) values and ion interaction parameters for Np(V) inorganic species are given along with their sources in Tables 5 and 6, respectively. Parameters that were taken from Fanghänel et al. (1995) or Neck et al. (1995) used a slightly different set of binary ion interaction parameters for carbonate species. The parameter values at issue are listed in Table 7, including the values from the Harvie et al. (1984) data base, as preferred for WIPP application, and the values from Pitzer (1991) used by Fanghänel et al. (1995) and Neck et al. (1995). Discussions with Dr. Volker Neck and Dr. Thomas Fanghänel of the Forschungszentrum Karlsruhe, Institut für Nukleare Entsorgungstechnik, and Dr. Andrew R. Felmy of Pacific Northwest National Laboratories led to the conclusion that these small differences in parameter values are unimportant and well within the accuracy of the solubility model. Therefore, we have taken the Np(V) parameters from Fanghänel et al. (1995) and Neck et al. (1995) directly without modification for use in the CHEMDAT data base file with parameters from Harvie et al. (1984). Documentation of the predictive ability of the Np(V) model in 0.8, 3.0, and 7.8m synthetic WIPP brines and in concentrated K-Cl-CO_3 and Na-K-Cl-CO_3 is in progress in Novak et al. (1996) and Al Mahamid et al. (1996).

References

Al Mahamid, I., C.F. Novak, K.A. Becraft, S.A. Carpenter, and N. Hakem. 1996. "Measurement and Thermodynamic Model Predictions of Np(V) Solubility in K_2CO_3/KCl and Na_2CO_3/KCl/NaCl Mixtures to High Concentration." manuscript in preparation.

Fanghänel, Th., J.I. Kim, P. Paviet, R. Klenze, and W. Hauser. 1994. "Thermodynamics of Radioactive Trace Elements in Concentrated Electrolyte Solutions: Hydrolysis of Cm^{3+} in NaCl Solutions." *Radiochimica Acta* vol. 66/67: 81-87.

Fanghänel, Th., V. Neck, and J.I. Kim. 1995. "Thermodynamics of Neptunium(V) in Concentrated Salt Solutions: II. Ion Interaction (Pitzer) Parameters for Np(V) Hydrolysis Species and Carbonate Complexes." *Radiochimica Acta* vol. 69: 169-173.

Felmy, A.R., and D. Rai. 1992. "An Aqueous Thermodynamic Model for a High Valence 4:2 Electrolyte Th^{4+}-SO_4^{2-} in the System Na^+-K^+-Li^+-NH_4^+-SO_4^{2-}-HSO_4^--H_2O to High Concentration." *Journal of Solution Chemistry* vol. 21 #5: 407-423.

Felmy, A.R., D. Rai, and R.W. Fulton. 1990. "The Solubility of $AmOHCO_3$(c) and the Aqueous Thermodynamics of the System Na^+-Am^{3+}-HCO_3^--OH^--H_2O." *Radiochimica Acta* vol. 50: 193-240.

Felmy, A.R., D. Rai, and M.J. Mason. 1991. "The Solubility of Hydrous Thorium(IV) Oxide in Chloride Media: Development of an Aqueous Ion-Interaction Model." *Radiochimica Acta* vol. 55: 177-185.

Felmy, A.R., D. Rai, J.A. Schramke, and J.L. Ryan. 1989. "The Solubility of Plutonium Hydroxide in Dilute Solution and in High-Ionic-Strength Chloride Brines." *Radiochimica Acta* vol. 48: 29-35.

Felmy, A.R., D. Rai, S.M. Sterner, M.J. Mason, N.J. Hess, and S.D. Conradson. 1996. "Thermodynamic Models for Highly Charged Aqueous Species: The Solubility of Th(IV) Hydrous Oxide in Concentrated $NaHCO_3$ and Na_2CO_3 Solutions." manuscript in preparation.

Felmy, A.R., and J.H. Weare. 1986. "The Prediction of Borate Mineral Equilibria in Natural Waters: Application to Searles Lake, California." *Geochimica et Cosmochimica Acta* vol. 50: 2771-2783.

Fuger, J. and F.L. Oetting. 1976. *The Chemical Thermodynamics of Actinide Elements and Compounds: Part 2. The Actinide Aqueous Ions.* Vienna, Austria: International Atomic Energy Agency.

Harvie, C.E., N. Møller, and J.H. Weare. 1984. "The Prediction of Mineral Solubilities in Natural Waters: The Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O System to High Ionic Strength at 25_C." *Geochimica et Cosmochimica Acta* vol. 48: 723-751.

Morss, L.R, and C.W. Williams. 1994. "Synthesis of Crystalline Americium Hydroxide, $Am(OH)_3$, and Determination of its Enthalpy of Formation; Estimation of the Solubility-Product Constants of Actinide(III) Hydroxides." *Radiochimica Acta* vol. 66/67: 89-93.

Neck., V. Th. Fanghänel, G. Rudolph and J.I. Kim. 1995. "Thermodynamics of Neptunium(V) in Concentrated Salt Solutions: Chloride Complexation and Ion Interaction (Pitzer) Parameters for the NpO_2^+ Ion." *Radiochimica Acta* vol. 69: 39-47.

Novak, C.F., I. Al Mahamid, K.A. Becraft, S.A. Carpenter, N. Hakem, and T. Prussin. 1996. "Measurement and Thermodynamic Modeling of Np(V) Solubility in Dilute Through Concentrated K_2CO_3 Media." manuscript in preparation.

Pitzer, K.S. 1991. "Ion Interaction Approach: Theory and Data Correlation." Chapter 3, pp. 75-153 in *Activity Coefficients in Electrolyte Solutions*. K.S. Pitzer, editor. Boca Raton, Florida: CRC Press.

Rai, D., A.R. Felmy, and R.W. Fulton. 1992. "Solubility and Ion Activity Product of $AmPO_4 \cdot xH_2O$(am)." *Radiochimica Acta* vol. 56: 7-14.

Rai, D., A.R. Felmy, and R.W. Fulton. 1995. "The Nd^{3+} and Am^{3+} Ion Interactions with Sulfate Ion and their Influence on $NdPO_4$(c) Solubility." *Journal of Solution Chemistry*. vol. 24 no. 9: 879-895.

Rai, D., A.F. Felmy, S.M. Sterner, D.A. Moore, M.J. Mason, and C.F. Novak. 1996. "The Solubility of Th(IV) and U(IV) Hydrous Oxides in Concentrated NaCl and $MgCl_2$ Solutions." *Radiochimica Acta* in press.

Rao, L., D. Rai, A.R. Felmy, RW. Fulton, and C.F. Novak. 1996a. "Solubility of $NaNd(CO_3)_2 \cdot 6H_2O$ in Concentrated Sodium Carbonate and Sodium Bicarbonate Solutions." *Radiochimica Acta* in press.

Rao, L., et al. 1996b. "Solubility of $NaNd(CO_3)_2 \cdot 6H_2O$ in Concentrated Sodium-Carbonate-Chloride and Sodium-Bicarbonate-Chloride Solutions." manuscript in preparation.

Roy, R.N., K.M. Vogel, C.E. Good, W.B. Davis, L.N. Roy, D.A. Johnson, A.R. Felmy, and K.S. Pitzer. 1992. "Activity Coefficients in Electrolyte Mixtures: HCl + $ThCl_4$ + H_2O for 5_–55_C." *Journal of Physical Chemistry* vol. 96: 11065-11072.

Runde, W., and J.I. Kim. 1995. *Chemical Behavior of Trivalent and Pentavalent Americium in Saline NaCl Solutions*. RCM 01094. Munich, Germany: Institute for Radiochemistry, Technical University of Munich. copy of the original (in German) and the English translation on file in the Sandia WIPP Central Files.

Silva, R.J., G. Bidoglio, M.H. Rand, P.B. Robouch, H. Wanner, and I. Puigdomenech. 1995. *Chemical Thermodynamics of Americium*. Elsevier Science Publishers: Amsterdam, The Netherlands.

Distribution:

SWCF-A: 1.1.10.1.1: PDD: QA: Data from Thermodynamic Predictions of Actinide Solubilities: WPO 38628

6831 R.V. Bynum, MS 1320

6831 E.J. Nowak, MS 1320

6832 S.C. Babb, MS 1341

6832 C.C. Crafts, MS 1341

6832 J.T. Holmes, MS 1341

6832 C.F. Novak, MS 1320

Table 1. Dimensionless standard chemical potentials for Am(III) and Pu(III) species.

Species	$\frac{\mu^\circ}{RT}$	Source
Am^{3+}	–241.694	Felmy et al., 1990
$AmCO_3^+$	–472.060	Felmy et al., 1990
$Am(CO_3)_2^-$	–695.880	Felmy et al., 1990
$Am(CO_3)_3^{3-}$	–915.460	Felmy et al., 1990
$AmOH^{2+}$	–315.352	Appendix A
$Am(OH)_2^+$	–392.281	Appendix A
$Am(OH)_3(aq)$	–471.603	Appendix A
$AmOHCO_3(s)$	–569.980	Felmy et al., 1990
$Am(OH)_3(s)$	–492.294	Felmy et al., 1989
$NaAm(CO_3)_2 \cdot 6H_2O(c)$	–1154.800	Rao et al., 1996
$AmPO_4(c)$	–709.750	Rai et al., 1992
Pu^{3+}	–233.4	Felmy et al., 1989
$PuCO_3^+$	–463.766	Felmy et al., 1990
$Pu(CO_3)_2^-$	–687.586	Felmy et al., 1990
$Pu(CO_3)_3^{3-}$	–907.166	Felmy et al., 1990

Species	$\frac{\mu^\circ}{RT}$	Source
$PuOH^{2+}$	–307.058	Appendix A
$Pu(OH)_2^+$	–383.987	Appendix A
$Pu(OH)_3(aq)$	–463.309	Appendix A
$PuOHCO_3(s)$	–561.686	Felmy et al., 1990
$Pu(OH)_3(s)$	–484.000	Felmy et al., 1989
$NaPu(CO_3)_2 \cdot 6H_2O(c)$	–1388.174	Rao et al., 1996
$PuPO_4(c)$	–701.456	Rai et al., 1992

Table 2. Ion interaction parameters for Am(III) and Pu(III) species. Parameters for Pu(III), not explicitly listed, are identical. Parameters not listed are zero.

Binary Interaction Parameters

i	j	$\beta_{ij}^{(0)}$	$\beta_{ij}^{(1)}$	$\beta_{ij}^{(2)}$	C_{ij}^{ϕ}	Source
Na^+	$Am(CO_3)_3^{3-}$	–0.256	5.0	0	0.0443	Rao et al., 1996
Am^{3+}	Cl^-	0.6117	5.403	0	–0.0284	Felmy et al., 1989
Am^{3+}	SO_4^{2-}	3.0398	0	–2500	0	Rai et al., 1995
Am^{3+}	ClO_4^-	0.80	5.35	0	–0.0048	Felmy et al., 1990
Am^{3+}	$H_2PO_4^-$	0	0	–92.9	0	Rai et al., 1995
$AmOH^{2+}$	Cl^-	–0.6	3.0	0	0.2	Fanghänel et al., 1994
$Am(OH)_2^+$	Cl^-	–0.58	–0.9	0	0	Fanghänel et al., 1994

Ternary Interaction Parameters

i	j	k	θ_{ij}	Ψ_{ijk}	Source
$Am(CO_3)_3^{3-}$	Cl^-	-	0.16	-	Rao et al., 1996b
SO_4^{2-}	ClO_4^-	Na+	0.020	0.0014	Rai et al., 1995

Table 3. Dimensionless standard chemical potentials for Th(IV) species.

Species	$\frac{\mu^\circ}{RT}$	Source
Th^{4+}	–284.227	Felmy et al., 1991
$Th(CO_3)_5^{6-}$	–1411.378@	Felmy et al., 1996
$Th(OH)_3CO_3^-$	–775.627*	Felmy et al., 1996
$Th(OH)_4(aq)$	–622.840	Andy Felmy, personal communication
$Th(SO_4)_2(aq)$	–911.69	Felmy and Rai, 1992
$Th(SO_4)_3^{2-}$	–1214.0	Felmy and Rai, 1992
$ThO_2(am)$	–451.408#	Felmy et al., 1991
$Th(SO_4)_2 \cdot 9H_2O(s)$	–1775.90	Felmy and Rai, 1992
$Th(SO_4)_2 \cdot 8H_2O(s)$	–1680.00	Felmy and Rai, 1992
$Th(SO_4)_2 \cdot Na_2SO_4 \cdot 6H_2O(s, 16\_C)$	–2011.29	Felmy and Rai, 1992
$Th(SO_4)_2 \cdot K_2SO_4 \cdot 4H_2O(s, 16\_C)$	–1837.57	Felmy and Rai, 1992
$Th(SO_4)_2 \cdot 2K_2SO_4 \cdot 2H_2O(s, 16\_C)$	–2181.81	Felmy and Rai, 1992
$Th(SO_4)_2 \cdot 3.5K_2SO_4(s, 16\_C)$	–2790.83	Felmy and Rai, 1992

@ = $-[\ \ln(10^{37.6}) - (-451.408) - 4(0.0) - 5(-212.944) + 2(95.6635)]$, compare with second reaction in Table 1 of Felmy et al., 1996

* = $-[\ \ln(10^{6.78}) - (-451.408) - 0.0 - (95.6635) - (-212.944)\ ]$, compare with first reaction in Table 1 of Felmy et al., 1996

= $-[\ -\ln(10^{-45.5}) - (-284.227) - 4(-63.435) + 2(-95.6635)\ ]$, compare with reaction on p. 182 of Felmy et al., 1991

Table 4. Ion interaction parameters for Th(IV) species. Parameters not listed or marked "-" are zero.

Binary Interaction Parameters

i	j	$\beta_{ij}^{(0)}$	$\beta_{ij}^{(1)}$	$\beta_{ij}^{(2)}$	C_{ij}^{ϕ}	Source
Na^+	ClO_4^-	0.0554	0.2755	0.0	–0.00118	Pitzer, 1991
Na+	$Th(CO_3)_5^{6-}$	1.31	30.0	-	-	Felmy et al., 1996
Na^+	$Th(SO_4)_3^{2-}$	0.12	-	-	-	Felmy and Rai, 1992
K^+	$Th(SO_4)_3^{2-}$	0.90	-	-	-	Felmy and Rai, 1992
H^+	ClO_4^-	0.1747	0.2931	0.0	0.00819	Pitzer, 1991
H^+	$Th(SO_4)_3^{2-}$	0.84	-	-	-	Felmy and Rai, 1992
Th^{4+}	Cl^-	1.092	13.7	–160.0	-0.112	Roy et al., 1992
Th^{4+}	SO_4^{2-}	1.56	-	-	-	Felmy and Rai, 1992
Th^{4+}	HSO_4^-	1.44	-	-	-	Felmy and Rai, 1992

Ternary Interaction Parameters

i	j	k	θ_{ij}	Ψ_{ijk}	Source
Na^+	Th^{4+}	Cl^-	0.42	0.21	Rai et al., 1996
Mg^{2+}	Th^{4+}	Cl^-	0.60	0.21	Rai et al., 1996

H^+	Th^{4+}	Cl^-	0.60	0.37	Roy et al., 1992
Cl^-	$Th(CO_3)_5^{6-}$	-	5.5	-	by analogy with ClO_4^-
ClO_4^-	$Th(CO_3)_5^{6-}$	-	5.5	-	Felmy et al., 1996

Neutral Interaction Parameters

n	i	λ_{ni}	Source
$Th(SO_4)_2(aq)$	Cl^-	0.29	Felmy and Rai, 1992
$Th(SO_4)_2(aq)$	HSO_4^-	0.68	Felmy and Rai, 1992

Appendix V: Memorandum on Current Release of Data Base

Table 5. Dimensionless standard chemical potential values for Np(V) species.

Species	$\frac{\mu^\circ}{RT}$	Source
NpO_2^+	–369.109	Fuger and Oetting, 1976
$NpO_2CO_3^-$	–593.635	Fanghänel et al., 1995
$NpO_2(CO_3)_2^{3-}$	–809.895	Fanghänel et al., 1995
$NpO_2(CO_3)_3^{5-}$	–1020.306	Fanghänel et al., 1995
$NpO_2OH(aq)$	–438.738	Fanghänel et al., 1995
$NpO_2(OH)_2^-$	–506.249	Fanghänel et al., 1995
$NaNpO_2CO_3(s)$	–712.871	Fanghänel et al., 1995
$NaNpO_2CO_3 \cdot 3.5H_2O(s)$	–1048.062	Fanghänel et al., 1995
$Na_3NpO_2(CO_3)_2(s)$	–1144.601	Fanghänel et al., 1995
$NpO_2OH(am)$	–452.761	Fanghänel et al., 1995
$NpO_2OH(aged)$	–454.373	Fanghänel et al., 1995
$KNpO_2CO_3(s)$	–727.33	Novak et al., 1996
$K_3NpO_2(CO_3)_2(s)$	–1173.55	Novak et al., 1996

Table 6. Ion interaction parameters for Np(V) species. Parameters not listed are zero.

Binary Interaction Parameters

i	j	$\beta_{ij}^{(0)}$	$\beta_{ij}^{(1)}$	$\beta_{ij}^{(2)}$	C_{ij}^{ϕ}	Source
NpO_2^+	Cl^-	0.1415	0.281	0	0	Fanghänel et al., 1995
NpO_2^+	ClO_4^-	0.257	0.180	0	0.0081	Fanghänel et al., 1995
Na^+	$NpO_2(OH)_2^-$	0	0	0	0	Fanghänel et al., 1995
Na^+	$NpO_2CO_3^-$	0.10	0.34	0	0	Fanghänel et al., 1995
Na^+	$NpO_2(CO_3)_2^{3-}$	0.48	4.4	0	0	Fanghänel et al., 1995
Na^+	$NpO_2(CO_3)_3^{5-}$	1.80	22.7	0	0	Fanghänel et al., 1995
K^+	$NpO_2CO_3^-$	0.10	0.34	0	0	Novak et al., 1996
K^+	$NpO_2(CO_3)_2^{3-}$	0.48	4.4	0	0	Novak et al., 1996
K^+	$NpO_2(CO_3)_3^{5-}$	2.34	22.7	–96.	–0.22	Novak et al., 1996

Ternary Interaction Parameters

i	j	k	θ_{ij}	Ψ_{ijk}	Source
OH^-	ClO_4^-	-	–0.032	-	Neck et al., 1995a

HCO_3^-	ClO_4^-	Na^+	0.095	–0.010	Neck et al., 1995a
CO_3^{2-}	ClO_4^-	Na^+	0.21	–0.024	Neck et al., 1995a
$NpO_2(OH)_2^-$	Cl^-	-	–0.24	-	Fanghänel et al., 1995
$NpO_2CO_3^-$	Cl^-	-	–0.21	-	Fanghänel et al., 1995
$NpO_2(CO_3)_2^{3-}$	Cl^-	-	–0.26	-	Fanghänel et al., 1995
$NpO_2(CO_3)_3^{5-}$	Cl^-	-	–0.26	-	Fanghänel et al., 1995
$NpO_2(CO_3)_3^{5-}$	CO_3^{2-}	-	–1.9	-	Novak et al., 1996

Neutral Interaction Parameters

n	i	λ_{ni}	Source
$NpO_2OH(aq)$	Na^+	0	Fanghänel et al., 1995
$NpO_2OH(aq)$	Cl^-	–0.19	Fanghänel et al., 1995

Table 7. Binary ion interaction parameters values from Harvie et al. (1984) used in the WIPP data base, and from Pitzer (1991) used to develop Np(V) parameter values in Fanghänel et al. (1995) and Neck et al (1995).

i	j	$\beta_{ij}^{(0)}$	$\beta_{ij}^{(1)}$	$\beta_{ij}^{(2)}$	Source
Na^+	CO_3^{2-}	0.0399	1.389	0.0044	Harvie et al., 1984
Na^+	CO_3^{2-}	0.0362	1.510	0.0052	Pitzer, 1991
Na^+	HCO_3^-	0.0277	0.0411	0	Harvie et al., 1984
Na^+	HCO_3^-	0.028	0.044	0	Pitzer, 1991

Appendix A: Parameter Values for +III Actinide Hydrolysis Species

This appendix documents thermodynamic parameters for the first, second, and third +III actinide hydrolysis species, here represented by americium: $AmOH^{2+}$, $Am(OH)_2^+$, and $Am(OH)_3(aq)$. As stated by Silva et al. (1995, p. 80) "there is no experimental evidence for anionic hydrolysis complexes of Am(III)." By chemical analogy, it is assumed that this applies to the other +III actinides as well. Hydrolysis species can be the dominant aqueous forms of +III actinides under conditions where more strongly complexing anions like the carbonate ion are absent. Hydrolysis species become more important as the hydroxide ion concentration is increased, i.e., as pH is increased.

The hydrolysis of Am(III) is given by

$$Am^{3+} + nOH^- \leftrightarrow Am(OH)_n^{3-n} \qquad \beta_{1n}^- = \frac{{}^a Am(OH)_n^{3-n}}{{}^a Am^{3+}\ {}^a OH^{-n}} \qquad \text{(A-1)}$$

and the solubility of americium hydroxide is given by

$$Am(OH)_3(s) \leftrightarrow Am^{3+} + 3\ OH^- \qquad K_{sp}^- = {}^a Am^{3+}\ {}^a OH^{-3} \qquad \text{(A-2)}$$

The ion interaction parameters between the first and second Cm(III) hydrolysis species and the chloride ion were reported by Fanghänel et al. (1994). These binary interaction parameters are given in Table 2 in the main text. We apply these values directly to Am(III) hydrolysis species without modification.

Literature values for the stability constants for the hydrolysis species, Equation A-1, and the solubility product for the hydroxide solid, Equation A-2, are presented in Table A-1. In order to maintain a consistent data base, the constants for the hydrolysis species must be modified for use with the $Am(OH)_3(s)$ solubility product in the CHEMDAT data base. Consistency will be maintained by requiring that the constants associated with the sum of the above reactions be the same, i.e.,

$$Am(OH)_3(s) \leftrightarrow Am(OH)_n^{3-n} + (3-n)\ OH^-$$

$$\beta_{1n}^- K_{sp}^- = a_{Am(OH)_n^{3-n}}\ a_{OH^-}^{(3-n)} \qquad \text{(A-3)}$$

The data base uses the solubility product value –26.2 from the value for $Pu(OH)_3(s)$ (Felmy et al., 1989). Fanghänel et al. (1994) use the value for $Am(OH)_3(s)$ of $\log K_{sp}^- = -28.2$ reported by Morss and Williams (1994). To maintain consistency within the data base, we continue to use the value from Felmy et al. (1989). In future refinements, the data base may benefit from reexamination of this parameter value assignment.

Because Fanghänel et al. (1994) do not report a value for the third hydrolysis constant, the value was arrived by the following method. Runde and Kim (1995) present measurements of the solubility of $Am(OH)_3(s)$ in 5M NaCl media. These data for pH>11 average 9.2×10^{-10}M, or 1.03×10^{-9}m total Am(III) solubility under these conditions where the third hydrolysis species is the dominant form of Am(III) in solution. We have rounded this to a limiting aqueous concentration of 1×10^{-9}m in 5.6m NaCl. Ion interaction parameters between the third hydrolysis species and Na^+ or Cl^- have apparently not been reported. Assuming that the activity of the neutral third hydrolysis species is little influenced by the solution composition or ionic strength, we assigned the value zero to all ion interaction parameters for this species, and achieved the equilibrium constant value reported in Table A-1. The equilibrium constants converted to dimensionless standard chemical potential values are given in Table 1 in the main text.

Table A-1. Thermodynamic stability constants for +III actinide hydrolysis species and $An(OH)_3(s)$

$\log\beta_{11}^-$	$\log\beta_{12}^-$	$\log\beta_{13}^-$	$\log K_{sp}^-$	Reference
6.44±0.09	12.3±0.2	n/d	–28.2	Fanghänel et al., 1994
7.59±0.7	13.88±0.6	16.27±0.5		Silva et al., 1995
n/d	n/d	n/d	–26.2	Felmy et al., 1989
4.44*	10.3*	17.2*	–26.2	values used in data base

* calculated as indicated in text; n/d=not determined

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
'HMW_Am3Pu3Th4Np2.CHEMDAT:  Am(III), Pu(III), Th(IV), Np(V)'
'96.08.23 Memo Release      HMW/FW; Ac-Cit-EDTA-Lac-Ox; MgOH2-CaOH2'

27 210 'nNEM T' 'nACTCOEF' 'nECHO' 'nABCD'
200 1.d-6 1.d-18
'NONE' 298.15 1.d0 1.d0

'Hydrogen' 'Oxygen' 'Sodium' 'Potassium' 'Magnesium' 'Calcium' 'Chlorine' 'Sulfur' 'Carbon' 'PosIon:EL'
   'NegIon:EL' 'Oxalate:EL' 'Boron' 'Bromine' 'Acetate:EL' 'Th(IV)' 'Am(III)' 'Pu(III)' 'Np(V)'
   'Cl04:EL' 'Phosphorus' 'U(IV)' 'Lactate:EL' 'EDTA:EL' 'Citrate:EL' 'Electron:EL' 'Charge:EL'
1.0079 15.9994 22.98977 39.0983 24.305 40.08 35.453 32.06 12.011 0.0 0.0 28.84 10.81 79.904 59.044
   232.0381 243.0 238.029 237.0482 99.4506 30.974 242.0 89.07 888.888 189.1 0.0 0.0

'H2O                    WATER'  2  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0 95.6635    HMW84
'Na+                      Na+'  0  0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1  1 -105.651  HMW84
'K+                        K+'  0  0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1  1 -113.957  HMW84
'Ca++                    Ca++'  0  0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2  1 -223.30   HMW84
'Mg++                    Mg++'  0  0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2  1 -183.468  HMW84
'MgOH+                  MgOH+'  1  1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1  1 -251.94   HMW84
'H+                        H+'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1  1  0.       HMW84

'Cl-                      Cl-'  0  0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1  1 -52.955  HMW84
'SO4=                    SO4='  0  4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2  1 -300.386 HMW84
'HSO4-                  HSO4-'  1  4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1  1 -304.942 HMW84
'OH-                    OH-'    1  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1  1 -63.435  HMW84
'HCO3-                  HCO3-'  1  3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1  1 -236.751 HMW84
'CO3=                    CO3='  0  3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2  1 -212.944 HMW84

'CO2(aq)              CO2(aq)'  0  2 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0  1 -155.68  HMW84
'CaCO3(aq)          CaCO3(aq)'  0  3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0  1 -443.5   HMW84
'MgCO3(aq)          MgCO3(aq)'  0  3 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0  1 -403.155 HMW84

'B(OH)3(aq)        B(OH)3(aq)'  3  3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0  0  1 -390.81  FWB6
'B(OH)4-            B(OH)4-'    4  4 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 -1  1 -465.20  FWB6
'B3O3(OH)4-        B3O3(OH)4-'  4  7 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1  1 -963.77  FWB6
'B4O5(OH)4=        B4O5(OH)4='  4  9 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2  1 -1239.10 FWB6
'CaB(OH)4+        CaB(OH)4+'    4  4 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1  1 -692.30  FWB6
'MgB(OH)4+        MgB(OH)4+'    4  4 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1  1 -651.89  FWB6
'Br-                      Br-'  0  0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 -1  1 -999.99  Arbitrary
'Cl04-                perchlorate'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 -1  1 -73.81  CFN950705

'NaOH(aq)       to.titrate.base.only'  1  1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0  1  500.  arbitrary
'HCl(aq)        to.titrate.acid.only'  1  0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0  1  500.  arbitrary
'HCl04(aq)      to.titrate.acid.only'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  0  1  500.  arbitrary
'PosIon                POSITIVE.ION'  0  0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1  1  0.    arbitrary
'NegIon                NEGATIVE.ION'  0  0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1  1  0.    arbitrary
'PosIon(OH)(aq)  to.titrate.base'     1  1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0  1  500.  arbitrary
'NNegIon(aq)     to.titrate.acid'     1  0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0  1  500.  arbitrary

'H3PO4(aq)            H3PO4(aq)'  3  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  0  1 -460.90  RFF92
'H2PO4-                H2PO4-'    2  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 -1  1 -455.96  RFF92
'HPO4=                  HPO4='    1  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 -2  1 -439.367 CFN95a
'PO4=                   PO4='     0  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 -3  1 -410.947 RFF94

'Am+++                  Am+++'    0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  3  1 -241.694  FRF90
'AmCO3+                AmCO3+'    0  3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  1  1 -472.060  FRF90
'Am(CO3)2-          Am(CO3)2-'    0  6 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -1  1 -695.880  FRF90
'Am(CO3)3=          Am(CO3)3='    0  9 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -3  1 -915.460  FRF90
'AmOH++      (after_Cm(III))'     1  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  2  1 -315.352
'Am(OH)2+    (after_Cm(III))'     2  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  1  1 -392.281
'Am(OH)3(aq) (1e-9m_minimum)'     3  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  0  1 -471.603

'Pu+++                  Pu+++'    0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  3  1 -233.4   FRSR89
'PuCO3+                PuCO3+'    0  3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  1  1 -463.766  analogy w/Am(III)
'Pu(CO3)2-          Pu(CO3)2-'    0  6 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -1  1 -687.586  analogy w/Am(III)
'Pu(CO3)3=          Pu(CO3)3='    0  9 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -3  1 -907.166  analogy w/Am(III)
'PuOH++      (after_Cm(III))'     1  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  2  1 -307.058  analogy w/Am(III)
'Pu(OH)2+    (after_Cm(III))'     2  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  1  1 -381.987  analogy w/Am(III)
'Pu(OH)3(aq) (1e-9m_minimum)'     3  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  0  1 -463.309  analogy w/Am(III)

'Th++++                 Th++++'   0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  4  1 -284.227  FRM91
'Th(CO3)5===         Th(CO3)5==='  0 15 0 0 0 0 0 0 5 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 -6  1 -1411.378 FRSMHC96
'Th(OH)3(CO3)-     Th(OH)3(CO3)-'  3  6 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 -1  1 -775.627  FRSMHC96
'Th(OH)4(aq)         Th(OH)4(aq)'  4  4 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  0  1 -622.840  CFN960119
'Th(SO4)2(aq)       Th(SO4)2(aq)'  0  8 0 0 0 0 0 2 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  0  1 -911.69   FR92
'Th(SO4)3=           Th(SO4)3='    0 12 0 0 0 0 0 3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 -2  1 -1214.0   FR92

'U++++                  U++++'    0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  4  1 -214.19  RFSH00N
'UOH+++                UOH+++'    1  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  3  1 -308.7   RFSH00N
'U(CO3)5===         U(CO3)5==='   0 15 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -6  1 -1345.393 Ral96
'U(OH)2(CO3)2=   U(OH)2(CO3)2='   2  8 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -2  1 -863.383  Ral96
'U(OH)4(CO3)2==U(OH)4(CO3)2=='    4 10 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -4  1 -998.662  Ral96
'U(OH)4(aq)           U(OH)4(aq)' 4  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  0  1  999.999
'U(SO4)2(aq)         U(SO4)2(aq)' 0  8 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  0  1  999.999
'U(SO4)3=            U(SO4)3='    0 12 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 -3  1  999.999

'NpO2+                  NpO2+'    0  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0  1  1 -369.109  FNK95
'NpO2CO3-            NpO2CO3-'    0  5 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -1  1 -593.635  FNK95
'NpO2(CO3)2=      NpO2(CO3)2=-'    0  8 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -3  1 -809.895  FNK95
'NpO2(CO3)3==    NpO2(CO3)3==-'    0 11 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -5  1 -1020.306 FNK95
'NpO2OH(aq)         NpO2OH(aq)'  1  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  0  1 -438.738  FNK95
'NpO2(OH)2-         NpO2(OH)2-'  2  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 -1  1 -506.249  FNK95

'HAc(aq)              AceticAcid'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0  0  1 -158.1   NBC96
'Ac-                     Acetate-' 0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 -1  1 -147.347 NBC96

'H3Citrate(aq)      CitricAcid'  3  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0  1  000.000  RCM96
'H2Citrate-         H2Citrate-'  2  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -1  1   7.245  RCM96
'HCitrate=          HCitrate='   1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -2  1  18.3    RCM96
'Citrate=           Citrate=-'   0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -3  1  33.068  RCM96

'H4EDTA(aq)        H4EDTA(aq)'   4  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0  1  000.000  RCM96
'H3EDTA-            H3EDTA-'     3  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -1  1   5.360  RCM96
'H2EDTA=            H2EDTA='     2  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -2  1  11.659  RCM96
'HEDTA=-            HEDTA=-'     1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -3  1  26.700  RCM96
'EDTA==             EDTA=='      0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -4  1  52.109  RCM96

'H2Ox(aq)           OxalicAcid'  2  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0  1   0.000  RCM96
'HOx-               Bioxalate-'  1  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 -1  1   3.052  RCM96
'Ox=                Oxalate='    0  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 -2  1  12.790  RCM96

'HLactate(aq)       LacticAcid'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0  1  000.000  RCM96
'Lactate-              Lactate-' 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -1  1   9.002  RCM96

'AmAc++           AmAcetate++'    0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0  2  1 -395.358  RCM96
'AmCit(aq)      AmCitrate(aq)'    0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0  1  1 -228.687  RCM96
'AmEDTA-          AmEDTA-'        0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 -1  1 -232.977  RCM96
'AmOx+          AmOxalate+'       0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1  1 -243.403  RCM96
'AmLac++      AmLactate++'        0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0  2  1 -242.339  RCM96
```

```
'PuAc++                PuAcetate++'  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 2   1 -387.064    analogy w/Am(III)
'PuCit(aq)             PuCitrate(aq)' 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0   1 -220.393    analogy w/Am(III)
'PuEDTA-                  PuEDTA-'   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 -1   1 -226.683    analogy w/Am(III)
'PuOx+                 PuOxalate+'   0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1   1 -235.189    analogy w/Am(III)
'PuLac++               PuLactate++'  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 2   1 -234.045    analogy w/Am(III)

'ThAc+++               ThAc+++'      0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 3   1 -448.639    RCM96
'ThCit+                ThCit+'       0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 1 0 1   1 -285.706    RCM96
'ThEDTA(aq)            ThEDTA(aq)'   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0   1 -285.817    RCM96
'ThOx++                Th(C2O4)++'   0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 2   1 -297.076    RCM96
'ThLac+++              ThLac+++'     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 3   1 -291.182    RCM96

'UAc+++                U(IV)Ac+++'   0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 3   1 -378.602    analogy w/Th++++
'UCit+                 U(IV)Cit+'    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0   1 -215.669    analogy w/Th++++
'UEDTA(aq)             U(IV)EDTA(aq)' 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0   1 -215.780    analogy w/Th++++
'ULac+++               U(IV)Lac+++'  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0   1 -221.145    analogy w/Th++++
'UOx++                 U(IV)Ox++'    0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 2   1 -227.039    analogy w/Th++++

'NpO2Ac(aq)            NpO2Ac(aq)'   0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0   1 -519.809    NBC96
'NpO2Cit+              NpO2Citrate+' 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 -2   1 -343.066    RCM96
'NpO2EDTA+-            NpO2EDTA+-'   0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 -3   1 -337.03     RCM96b
'NpO2Ox-               NpO2Oxalate-' 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 -1   1 -366.452    RCM96
'NpO2Lac(aq)           NpO2Lactate(aq)' 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0   1 -364.266    RCM96

'HgAc+                 HgAc+'        0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1   1 -333.346    RCM96c
'HgCit-                HgCit-'       0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -1   1 -161.979    RCM96c
'HgEDTA=               HgEDTA='      0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -2   1 -160.325    RCM96c
'HgOx(aq)              HgOx(aq)'     0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0   1 -178.88     RCM96c
'HgLac+                HgLac+'       0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1   1  999.999

'CaAc+                 (Mg-analog)'  0 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1   1 -373.178    analogy w/Mg++
'CaCit-                (Mg-analog)'  0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -1   1 -201.811    analogy w/Mg++
'CaEDTA=               (Mg-analog)'  0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -2   1 -200.157    analogy w/Mg++
'CaOx(aq)              (Mg-analog)'  0 0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0   1 -218.712    analogy w/Mg++
'CaLac+                (Mg-analog)'  0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1   1  999.999

'UnuCat#1+             UC#1+'        0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1   1  999.999
'UnuAn#1-              UA#1-'        0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1  999.999
'UnuAn#2-              UA#2-'        0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1  999.999
'UnuAn#3-              UA#3-'        0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1  999.999
'UnuAn#4-              UA#4-'        0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1  999.999
'UnuNeu#1(aq)          UN#1(aq)'     0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   1  999.999

'AmOHCO3(c)_____AmOHCO3(c)'  1 4 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   2  -569.980    FRF90
'Am(OH)3(s)_____Am(OH)3(s)'  1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   2  -492.294
'NaAm(CO3)2.6H2O(c)_____'  12 12 1 0 0 0 0 0 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   2 -1396.468    RRFTH94
'AmPO4(c)_____AmPO4(c)'  0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0   2  -709.750    RFF92

'PuOHCO3(c)_____PuOHCO3(c)'  1 4 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   2  -561.686    analogy w/Am(III)
'Pu(OH)3(s)_____Pu(OH)3(s)'  3 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   2  -484.000    analogy w/Am(III)
'NaPu(CO3)2.6H2O(c)_____'  12 12 1 0 0 0 0 0 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   2 -1388.174    analogy w/Am(III)
'PuPO4(c)_____PuPO4(c)'  0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0 0   2  -701.456    analogy w/Am(III)

'ThO2(am)_____Hydrous_Thorium_Oxide'  0 2 0  0 0 0 0  0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  2 -451.408    FRM91
'Th(SO4)2.9H2O(s)_____'  18 17 0  0 0 0 0  2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  3 -1775.90    FR92
'Th(SO4)2.8H2O(s)_____'  16 16 0  0 0 0 0  2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  3 -1680.00    FR92
'Th(SO4)2.Na2SO4.6H2O(16C,s)_____'  12 18 2  0 0 0 0  3 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  3 -2011.29    FR92
'Th(SO4)2.K2SO4.4H2O(16C,s)_____'  8 16 0  2 0 0 0  3 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  3 -1837.57    FR92
'Th(SO4)2.2K2SO4.2H2O(16C,s)_____'  4 18 0  4 0 0 0  4 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  3 -2181.81    FR92
'2[Th(SO4)2.7/2K2SO4(16C,s)]_____'  0 44 0 14 0 0 0 11 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0  3 -5581.66 =2[-2790.83]    FR92

'UO2(am)_____Hydrous_U(IV)_Oxide'  0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  2 -399.67     RFSM90

'NpO2OH(aged)_____NpO2OH(aged)'  1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   2  -454.373    FNK95
'NpO2OH(amor)_____NpO2OH(amor)'  1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   2  -452.761    FNK95
'2[NaNpO2CO3.7/2H2O(s)]_____'  14 17 2 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0   2 -2096.124    =2*(-1048.062)  FNK95
'Na3NpO2(CO3)2(s)__Na3NpO2(CO3)2(s)'  0 8 3 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   2 -1144.601    FNK95
'KNpO2CO3(s)_____KNpO2CO3(s)'  0 5 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   2  -727.33     Np(V)MS1996
'K3Np02(CO3)2(s)____K3NpO2(CO3)2(s)'  0 8 0 3 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   2 -1173.55     Np(V)MS1996

'H2Ox.2H2O(s)_____H2C2O4.2H2O(s)'  6 2 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -191.370    CFN16APR96
'NaHOx.H2O(s)_____NaHC2O4.H2O(s)'  3 1 1 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -202.245    CFN16APR96
'Na2Ox(s)_____Na2C2O4(s)'  0 0 2 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -203.651    CFN16APR96
'CO2("solid",DISABLED)_____'  0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2  999.999    (-159.092 HMW)

'CaSO4_____Anhydrite'  0 4 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -533.73     HMW84
'NaK3(SO4)2__Aphthitalite/Glaserite'  0 8 1 3 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1057.05    HMW84
'CaCl2.6H2O_____Antarcticite'  12 6 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -893.65     HMW84
'CaCO3_____Aragonite'  0 3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -455.17     HMW84
'K2SO4_____Arcanite'  0 4 0 2 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -532.39     HMW84
'MgCl2.6H2O_____Bischofite'  12 6 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -853.1      HMW84
'Na2Mg(SO4)2.4H2O_____Bloedite'  8 12 2 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1383.6     HMW84
'Mg(OH)2_____Brucite'  2 2 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -335.4     HMW84
'Na6CO3(SO4)2_____Burkeite'  0 11 6 0 0 0 0 2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1449.4    HMW84
'CaCO3_____Calcite'  0 3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -455.6     HMW84
'CaCl2.4H2O_____CaCl2_Tetrahydrite'  8 4 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -698.7     HMW84
'Ca4Cl2(OH)6.13H2O___CaOxychloride_A'  32 19 0 0 0 4 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -2658.45    HMW84
'Ca2Cl2(OH)2.H2O____CaOxychloride_B'  4 3 0 0 0 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -778.41     HMW84
'KMgCl3.6H2O_____Carnallite'  12 6 0 1 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1020.3     HMW84
'MgSO4.7H2O_____Epsomite'  14 11 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1157.83    HMW84
'CaNa2(CO3)2.5H2O_____Gaylussite'  10 11 2 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1360.5     HMW84
'Na2Ca(SO4)2_____Glauberite'  0 8 2 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1047.45    HMW84
'CaSO4.2H2O_____Gypsum'  4 5 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -725.56     HMW84
'NaCl_____Halite'  0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -154.99     HMW84
'MgSO4.6H2O_____Hexahydrite'  12 10 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1061.60    HMW84
'KMgClSO4.3H2O_____Kainite'  5 7 0 1 1 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -938.2     HMW84
'KHCO3_____Kalicinite'  1 3 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -350.06    HMW84
'MgSO4.H2O_____Kieserite'  2 5 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -579.80    HMW84
'K2Mg(SO4)2.4H2O_____Leonite'  8 12 0 2 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1403.97    HMW84
'Na4Ca(SO4)3.2H2O_____Labile_Salt'  4 14 4 0 0 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1751.45    HMW84
'MgCO3_____Magnesite'  0 3 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -414.45    HMW84
'Mg2Cl(OH)3.4H2O_____MgOxychloride'  11 7 0 0 2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1029.6     HMW84
'KHSO4_____Mercallite'  1 1 4 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -417.57    HMW84
'Na2SO4.10H2O_____Mirabilite'  20 14 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1471.15    HMW84
'K8H6(SO4)7_____Misenite'  6 28 0 8 0 0 0 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -3039.24    HMW84
'NaHCO3_____Nahcolite'  1 3 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -343.33    HMW84
'Na2CO3.10H2O_____Natron'  20 13 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1382.78    HMW84
'MgCO3.3H2O_____Nesquehonite'  6 6 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -695.3     HMW84
'K2Mg(SO4)2.6H2O_Picromerite/Schoen'  12 14 0 2 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1596.1     HMW84
'Na2Ca(CO3)2.2H2O_____Pirssonite'  4 8 2 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1073.1     HMW84
'K2MgCa2(SO4)4.2H2O_____Polyhalite'  4 16 0 2 1 2 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -2282.5     HMW84
'Ca(OH)2_____Portlandite'  2 2 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -362.12    HMW84
'K2CO3.3/2H2O___Potassium_Carbonate'  3 4.5 0 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -577.37    HMW84
'K8H6(CO3)6.3H2O___K-Sequicarbonate'  10 21 0 8 0 0 0 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -2555.4     HMW84
'KNaCO3.6H2O_____K-Na-Carbonate'  12 9 1 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1006.8     HMW84
'K2NaH(CO3)2.2H2O___Potassium_Trona'  5 8 1 2 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -971.74     HMW84
'K3H(SO4)2___Sesquipotassium_Sulfate'  1 8 0 3 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -950.8     HMW84
'Na3H(SO4)2____Sesquisodium_Sulfate'  1 8 3 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -919.6     HMW84
'Na2CO3.7H2O____Na2CO3-Heptahydrate'  14 10 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1094.95    HMW84
'KCl_____Sylvite'  0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -164.84    HMW84
'K2Ca(SO4)2.H2O_____Syngenite'  2 9 0 2 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -1164.8     HMW84
'Mg2CaCl6.12H2O_____Tachyhydrite'  24 12 0 0 2 1 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -2015.9     HMW84
'Na2SO4_____Thenardite'  0 8 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -512.35    HMW84
'Na2CO3.H2O_____Thermonatrite'  2 4 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   2 -518.8     HMW84
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
'Na3H(CO3)2.2H2O_____________Trona'  5  8 3 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -960.38      HMW84
'Na2B4O7.10H2O_____________Borax' 20 17 2 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -3224.16     FW86
'B(OH)3_____Borix_Acid_Solid'  3  3 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -390.88      FW86
'KB5O8.4H2O____K-Pentaborate_(30_C)'  8 12 0 1 0 0 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1770.26     FW86
'K2B4O7.4H2O___K-Tetraborate_(30_C)'  8 11 0 2 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1663.47     FW86
'NaBO2.4H2O_____Sodium_Metaborate'  8  6 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -761.42      FW86
'NaB5O8.5H2O_____Sodium_Pentaborate' 10 13 1 0 0 0 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1054.80     FW86
'NaBO2.NaCl.2H2O___Teepleite_(20_C)'  4  4 2 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -725.77      FW86
'CaMg(CO3)2____DISABLED____Dolomite'  0  6 0 0 1 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 999.999 -871.99      HMW84

'nDG_BYPASS' 0
'PITZACT'
 39 #Cations
 53 #Anions
 26 #Neutrals

  1   .0765     .2644     .0     .00127   Na+ Cl-            HMW84 (beta0, beta1, beta2, cphi) NOTE: HMW gives .2644; P91 gives .2664
  1   .01958   1.113      .0     .00497   Na+ SO4=           HMW84
  1   .0454     .398      .0     .0       Na+ HSO4-          HMW84
  1   .0864     .253      .0     .0044    Na+ OH-            HMW84
  1   .0277     .0411     .0     .0       Na+ HCO3-          HMW84
  1   .0399    1.389      .0     .0044    Na+ CO3=           HMW84
  1 -.0427     .089      .0     .0114    Na+ B(OH)4-        FW86
  1 -.056     -.910      .0     .0       Na+ B3O3(OH)4-     FW86
  1 -.11      -.40       .0     .0       Na+ B4O5(OH)4=     FW86
  1   .0        .0       .0     .0       Na+ Br-
  1   .0        .0       .0     .0       Na+ Am(CO3)2-      RRFFN96
  1 -.256     5.0        .0     .0443    Na+ Am(CO3)3=-     RRFFN96
  1   .0554     .2755     .0    -.00118   Na+ ClO4-          P91
  1   .0        .0       .0     .0       Na+ NpO2(OH)2-     NR94/FNK95
  1   .10       .34      .0     .0       Na+ NpO2CO3-       FNK95
  1   .48      4.4       .0     .0       Na+ NpO2(CO3)2=-   FNK95
  1  1.80     22.7       .0     .0       Na+ NpO2(CO3)3=--  FNK95
  1 -.0533     .0396     .0     .00795   Na+ H2PO4-         P91
  1 -.0583    1.466      .0     .0294    Na+ HPO4=          P91
  1   .1781    3.851     .0    -.05154   Na+ PO4=-          P91
  1   .12       .0       .0     .0       Na+ Th(SO4)3=      FR92
  1   .0        .0       .0     .0       Na+ Th(OH)3(CO3)-
  1  1.31     30.        .0     .0       Na+ Th(CO3)5===    FRSMHC96
  1 -.0307     .0        .0     .0       Na+ HOx-           RCM96
  1  0.0028   1.661      .0     .027     Na+ Ox=            RCM96
  1   .1426     .22      .0    -.00629   Na+ Ac-            NBC96
  1   .1349    -.7242    .0     .0       Na+ Lac-           RCM96
  1 -0.0613    .5548     .0     .0       Na+ H2Cit-         RCM96
  1 -.0014    2.339      .0     .0       Na+ HCit=          RCM96
  1   .2823    5.411     .0     .0       Na+ Cit=-          RCM96
  1 -.0908     .0825     .0     .0       Na+ H3EDTA-        RCM96
  1 -.1272    2.863      .0     .0       Na+ H2EDTA=        RCM96
  1   .2619    8.325     .0     .0       Na+ HEDTA=-        RCM96
  1  1.034    11.36      .0     .0       Na+ EDTA==         RCM96
  1 -.2307     .0        .0     .0       Na+ AmEDTA=-       RCM96
  1 -.4092    1.221      .0     .213     Na+ NpO2Cit=       RCM96
  1   .5067    7.738     .0     .0       Na+ NpO2EDTA=-     RCM96b
  1 -.1893     .0        .0     .0       Na+ NpO2Ox-        RCM96
  1   .41     17.25      .0     .0       Na+ U(OH)4(CO3)2==  Rai96
  1  1.31     30.0       .0     .0       Na+ U(CO3)5===      Rai96
  1   .0        .0       .0     .0       Na+ U(SO4)3=
  1   .0        .0       .0     .0       Na+ Pu(CO3)2-      analogy w/Am(III)
  1 -.256     5.0        .0     .0443    Na+ Pu(CO3)3=-     analogy w/Am(III)
  1 -.2307     .0        .0     .0       Na+ PuEDTA=-       RCM96
  1   .2317    .0        .0     .0       Na+ CaCit-         analogy w/Mg++
  1   .9289    .0        .0     .0       Na+ CaEDTA=        analogy w/Mg++
  1   .0       .0        .0     .0       Na+ UnuAn#2-
  1   .0       .0        .0     .0       Na+ UnuAn#3-
  1   .0       .0        .0     .0       Na+ UnuAn#4-
  1   .0       .0        .0     .0       Na+ U(OH)2(CO3)2=
  1   .2317    .0        .0     .0       Na+ MgCit-          RCM96c
  1   .9289    .0        .0     .0       Na+ MgEDTA=         RCM96c
  1   .0       .0        .0     .0       Na+ UnuAn#1-

  1   .04835    .2122     .0    -.00084   K+ Cl-             HMW84
  1   .04995    .7793     .0     .0       K+ SO4=            HMW84
  1 -.0003     .1735     .0     .0       K+ HSO4-           HMW84
  1   .1298     .320      .0     .0041    K+ OH-             HMW84
  1   .0296    -.013      .0    -.008     K+ HCO3-           HMW84
  1   .1488    1.43       .0    -.0015    K+ CO3=            HMW84
  1   .035      .14       .0     .0       K+ B(OH)4-         FW86
  1 -.13       .0        .0     .0       K+ B3O3(OH)4-      FW86
  1 -.022      .0        .0     .0       K+ B4O5(OH)4=      FW86
  1   .0       .0        .0     .0       K+ Br-
  1   .0       .0        .0     .0       K+ Am(CO3)2-
  1   .0       .0        .0     .0       K+ Am(CO3)3=-
  1   .0       .0        .0     .0       K+ ClO4-
  1   .0       .0        .0     .0       K+ NpO2(OH)2-
  1   .10      .34       .0     .0       K+ NpO2CO3-        analogy w/Na+
  1   .48     4.4        .0     .0       K+ NpO2(CO3)2=-    analogy w/Na+
  1 2.34     22.7      -96.    -.22      K+ NpO2(CO3)3=--   Np(V)MS1996
  1 -.0678   -.1042     .0     .0       K+ H2PO4-          P91
  1   .0248    1.274    .0     .0164    K+ HPO4=           P91
  1   .3729    3.972    .0    -.08680   K+ PO4=-           P91
  1   .90       .0      .0     .0       K+ Th(SO4)3=       FR92
  1   .0        .0      .0     .0       K+ Th(OH)3(CO3)-
  1   .0        .0      .0     .0       K+ Th(CO3)5===
  1   .0        .0      .0     .0       K+ HOx-
  1   .0        .0      .0     .0       K+ Ox=
  1   .1587     .3251   .0    -.00660   K+ Ac-             P91
  1   .0        .0      .0     .0       K+ Lac-
  1   .0        .0      .0     .0       K+ H2Cit-
  1   .0        .0      .0     .0       K+ HCit=
  1   .0        .0      .0     .0       K+ Cit=-
  1   .0        .0      .0     .0       K+ H3EDTA-
  1   .0        .0      .0     .0       K+ H2EDTA=
  1   .0        .0      .0     .0       K+ HEDTA=-
  1   .0        .0      .0     .0       K+ EDTA==
  1   .0        .0      .0     .0       K+ AmEDTA=-
  1   .0        .0      .0     .0       K+ NpO2Cit=
  1   .0        .0      .0     .0       K+ NpO2EDTA=-
  1   .0        .0      .0     .0       K+ NpO2Ox-
  1   .41     17.25     .0     .0       K+ U(OH)4(CO3)2==  Rai96
  1  1.31     30.0      .0     .0       K+ U(CO3)5===      Rai96
  1   .0        .0      .0     .0       K+ U(SO4)3=
  1   .0        .0      .0     .0       K+ Pu(CO3)2-
  1   .0        .0      .0     .0       K+ Pu(CO3)3=-
  1   .0        .0      .0     .0       K+ PuEDTA-
  1   .0        .0      .0     .0       K+ CaCit-
  1   .0        .0      .0     .0       K+ CaEDTA=
  1   .0        .0      .0     .0       K+ UnuAn#2-
  1   .0        .0      .0     .0       K+ UnuAn#3-
  1   .0        .0      .0     .0       K+ UnuAn#4-
  1   .0        .0      .0     .0       K+ U(OH)2(CO3)2=
  1   .0        .0      .0     .0       K+ MgCit-
  1   .0        .0      .0     .0       K+ MgEDTA=
  1   .0        .0      .0     .0       K+ UnuAn#1-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
369     1  .3159     1.614      .0    -.00038   Ca++ Cl-            HMW84
370     2  .20       3.1973   -54.24    .0      Ca++ SO4=           HMW84
371     1  .2145     2.53       .0      .0      Ca++ HSO4-          HMW84
372     1 -.1747    -.2303    -5.72      .0      Ca++ OH-            HMW84
373     1  .4        2.977      .0      .0      Ca++ HCO3-          HMW84
374     2  .0         .0        .0      .0      Ca++ CO3=           HMW84
375     1  .0         .0        .0      .0      Ca++ B(OH)4-        FW86
376     1  .0         .0        .0      .0      Ca++ B3O3(OH)4-     FW86
377     2  .0         .0        .0      .0      Ca++ B4O5(OH)4=     FW86
378     1  .0         .0        .0      .0      Ca++ Br-
379     1  .0         .0        .0      .0      Ca++ Am(CO3)2-
380     3  .0         .0        .0      .0      Ca++ Am(CO3)3=-
381     1  .4511     1.756      .0    -.00500   Ca++ ClO4-          P91
382     1  .0         .0        .0      .0      Ca++ NpO2(OH)2-
383     1  .0         .0        .0      .0      Ca++ NpO2CO3-
384     3  .0         .0        .0      .0      Ca++ NpO2(CO3)2=-
385     3  .0         .0        .0      .0      Ca++ NpO2(CO3)3=5-
386     1  .0         .0        .0      .0      Ca++ H2PO4-
387     2  .0         .0        .0      .0      Ca++ HPO4=
388     3  .0         .0        .0      .0      Ca++ PO4=-
389     2  .0         .0        .0      .0      Ca++ Th(SO4)3=
390     1  .0         .0        .0      .0      Ca++ Th(OH)3(CO3)-
391     3  .0         .0        .0      .0      Ca++ Th(CO3)5===
392     1  .0         .0        .0      .0      Ca++ HOx-
393     2  .0         .0        .0      .0      Ca++ Ox=
394     1  .0         .0        .0      .0      Ca++ Ac-
395     1  .0         .0        .0      .0      Ca++ Lac-
396     1  .0         .0        .0      .0      Ca++ H2Cit-
397     2  .0         .0        .0      .0      Ca++ HCit=
398     3  .0         .0        .0      .0      Ca++ Cit=-
399     3  .0         .0        .0      .0      Ca++ H3EDTA-
400     3  .0         .0        .0      .0      Ca++ H2EDTA=
401     3  .0         .0        .0      .0      Ca++ HEDTA=-
402     3  .0         .0        .0      .0      Ca++ EDTA==
403     3  .0         .0        .0      .0      Ca++ AmEDTA=-
404     2  .0         .0        .0      .0      Ca++ NpO2Cit=
405     3  .0         .0        .0      .0      Ca++ NpO2EDTA==-
406     1  .0         .0        .0      .0      Ca++ NpO2Ox-
407     3  .0         .0        .0      .0      Ca++ U(OH)4(CO3)2==
408     3  .0         .0        .0      .0      Ca++ U(CO3)5===
409     2  .0         .0        .0      .0      Ca++ U(SO4)3=
410     1  .0         .0        .0      .0      Ca++ Pu(CO3)2-
411     2  .0         .0        .0      .0      Ca++ Pu(CO3)3=-
412     1  .0         .0        .0      .0      Ca++ PuEDTA-
413     1  .0         .0        .0      .0      Ca++ CaCit-
414     3  .0         .0        .0      .0      Ca++ CaEDTA=
415     3  .0         .0        .0      .0      Ca++ UmuAn#2-
416     1  .0         .0        .0      .0      Ca++ UmuAn#3-
417     3  .0         .0        .0      .0      Ca++ UmuAn#4-
418     2  .0         .0        .0      .0      Ca++ U(OH)2(CO3)2=
419     1  .0         .0        .0      .0      Ca++ MgCit-
420     2  .0         .0        .0      .0      Ca++ MgEDTA=
421     1  .0         .0        .0      .0      Ca++ UmuAn#1-
422
423     1  .35235    1.6815     .0      .00519  Mg++ Cl-            HMW84
424     2  .2210     3.343    -37.23    .025    Mg++ SO4=           HMW84
425     1  .4746     1.729      .0      .0      Mg++ HSO4-          HMW84
426     1  .0         .0        .0      .0      Mg++ OH-            HMW84
427     1  .329      .6072      .0      .0      Mg++ HCO3-          HMW84
428     2  .0         .0        .0      .0      Mg++ CO3=           HMW84
429     1  .0         .0        .0      .0      Mg++ B(OH)4-        FW86
430     1  .0         .0        .0      .0      Mg++ B3O3(OH)4-     FW86
431     2  .0         .0        .0      .0      Mg++ B4O5(OH)4=     FW86
432     1  .0         .0        .0      .0      Mg++ Br-
433     1  .0         .0        .0      .0      Mg++ Am(CO3)2-
434     3  .0         .0        .0      .0      Mg++ Am(CO3)3=-
435     1  .4961     2.008      .0      .009578 Mg++ ClO4-          P91
436     1  .0         .0        .0      .0      Mg++ NpO2(OH)2-
437     1  .0         .0        .0      .0      Mg++ NpO2CO3-
438     3  .0         .0        .0      .0      Mg++ NpO2(CO3)2=-
439     3  .0         .0        .0      .0      Mg++ NpO2(CO3)3=5-
440     1  .0         .0        .0      .0      Mg++ H2PO4-
441     2  .0         .0        .0      .0      Mg++ HPO4=
442     3  .0         .0        .0      .0      Mg++ PO4=-
443     2  .0         .0        .0      .0      Mg++ Th(SO4)3=
444     1  .0         .0        .0      .0      Mg++ Th(OH)3(CO3)-
445     3  .0         .0        .0      .0      Mg++ Th(CO3)5===
446     1  .0         .0        .0      .0      Mg++ HOx-
447     2  .0         .0        .0      .0      Mg++ Ox=
448     1  .0         .0        .0      .0      Mg++ Ac-
449     1  .0         .0        .0      .0      Mg++ Lac-
450     1  .0         .0        .0      .0      Mg++ H2Cit-
451     2  .0         .0        .0      .0      Mg++ HCit=
452     3  .0         .0        .0      .0      Mg++ Cit=-
453     3  .0         .0        .0      .0      Mg++ H3EDTA-
454     3  .0         .0        .0      .0      Mg++ H2EDTA=
455     3  .0         .0        .0      .0      Mg++ HEDTA=-
456     3  .0         .0        .0      .0      Mg++ EDTA==
457     3  .0         .0        .0      .0      Mg++ AmEDTA=-
458     2  .0         .0        .0      .0      Mg++ NpO2Cit=
459     3  .0         .0        .0      .0      Mg++ NpO2EDTA==-
460     1  .0         .0        .0      .0      Mg++ NpO2Ox-
461     3  .0         .0        .0      .0      Mg++ U(OH)4(CO3)2==
462     3  .0         .0        .0      .0      Mg++ U(CO3)5===
463     2  .0         .0        .0      .0      Mg++ U(SO4)3=
464     1  .0         .0        .0      .0      Mg++ Pu(CO3)2-
465     2  .0         .0        .0      .0      Mg++ Pu(CO3)3=-
466     1  .0         .0        .0      .0      Mg++ PuEDTA-
467     1  .0         .0        .0      .0      Mg++ CaCit-
468     3  .0         .0        .0      .0      Mg++ CaEDTA=
469     3  .0         .0        .0      .0      Mg++ UmuAn#2-
470     1  .0         .0        .0      .0      Mg++ UmuAn#3-
471     2  .0         .0        .0      .0      Mg++ UmuAn#4-
472     2  .0         .0        .0      .0      Mg++ U(OH)2(CO3)2=
473     1  .0         .0        .0      .0      Mg++ MgCit-
474     2  .0         .0        .0      .0      Mg++ MgEDTA=
475     1  .0         .0        .0      .0      Mg++ UmuAn#1-
476
477     1 -.10      1.658      .0      .0      MgOH+ Cl-           HMW84
478     1  .0         .0        .0      .0      MgOH+ SO4=          HMW84
479     1  .0         .0        .0      .0      MgOH+ HSO4-         HMW84
480     1  .0         .0        .0      .0      MgOH+ OH-           HMW84
481     1  .0         .0        .0      .0      MgOH+ HCO3-         HMW84
482     1  .0         .0        .0      .0      MgOH+ CO3=          HMW84
483     1  .0         .0        .0      .0      MgOH+ B(OH)4-
484     1  .0         .0        .0      .0      MgOH+ B3O3(OH)4-
485     1  .0         .0        .0      .0      MgOH+ B4O5(OH)4=
486     1  .0         .0        .0      .0      MgOH+ Br-
487     1  .0         .0        .0      .0      MgOH+ Am(CO3)2-
488     1  .0         .0        .0      .0      MgOH+ Am(CO3)3=-
489     1  .0         .0        .0      .0      MgOH+ ClO4-
490     1  .0         .0        .0      .0      MgOH+ NpO2(OH)2-
491     1  .0         .0        .0      .0      MgOH+ NpO2CO3-
492     1  .0         .0        .0      .0      MgOH+ NpO2(CO3)2=-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
493     1  .0        .0        .0        .0       MgOH+ NpO2(CO3)3=-
494     1  .0        .0        .0        .0       MgOH+ H2PO4-
495     1  .0        .0        .0        .0       MgOH+ HPO4=
496     1  .0        .0        .0        .0       MgOH+ PO4=-
497     1  .0        .0        .0        .0       MgOH+ Th(SO4)3=
498     1  .0        .0        .0        .0       MgOH+ Th(OH)3(CO3)-
499     1  .0        .0        .0        .0       MgOH+ Th(CO3)5===
500     1  .0        .0        .0        .0       MgOH+ HOx-
501     1  .0        .0        .0        .0       MgOH+ Ox=
502     1  .0        .0        .0        .0       MgOH+ Ac-
503     1  .0        .0        .0        .0       MgOH+ Lac-
504     1  .0        .0        .0        .0       MgOH+ H2Cit-
505     1  .0        .0        .0        .0       MgOH+ HCit=
506     1  .0        .0        .0        .0       MgOH+ Cit=-
507     1  .0        .0        .0        .0       MgOH+ H3EDTA-
508     1  .0        .0        .0        .0       MgOH+ H2EDTA=
509     1  .0        .0        .0        .0       MgOH+ HEDTA=-
510     1  .0        .0        .0        .0       MgOH+ EDTA==
511     1  .0        .0        .0        .0       MgOH+ AmEDTA=-
512     1  .0        .0        .0        .0       MgOH+ NpO2Cit=
513     1  .0        .0        .0        .0       MgOH+ NpO2EDTA==-
514     1  .0        .0        .0        .0       MgOH+ NpO2Ox-
515     1  .0        .0        .0        .0       MgOH+ U(OH)4(CO3)2=-
516     1  .0        .0        .0        .0       MgOH+ U(CO3)5===
517     1  .0        .0        .0        .0       MgOH+ U(SO4)3=
518     1  .0        .0        .0        .0       MgOH+ Pu(CO3)2-
519     1  .0        .0        .0        .0       MgOH+ Pu(CO3)3=-
520     1  .0        .0        .0        .0       MgOH+ PuEDTA-
521     1  .0        .0        .0        .0       MgOH+ CaCit-
522     1  .0        .0        .0        .0       MgOH+ CaEDTA=
523     1  .0        .0        .0        .0       MgOH+ UnuAn#2-
524     1  .0        .0        .0        .0       MgOH+ UnuAn#3-
525     1  .0        .0        .0        .0       MgOH+ UnuAn#4-
526     1  .0        .0        .0        .0       MgOH+ U(OH)2(CO3)2=
527     1  .0        .0        .0        .0       MgOH+ MgCit-
528     1  .0        .0        .0        .0       MgOH+ MgEDTA=
529     1  .0        .0        .0        .0       MgOH+ UnuAn#1-
530
531     1  .1775     .2965     .0        .0008    H+ Cl-                HMW84
532     1  .0298     .0        .0        .0438    H+ SO4=               HMW84
533     1  .2065     .5556     .0        .0       H+ HSO4-              HMW84
534     1  .0        .0        .0        .0       H+ OH-                HMW84
535     1  .0        .0        .0        .0       H+ HCO3-              HMW84
536     1  .0        .0        .0        .0       H+ CO3=               HMW84
537     1  .0        .0        .0        .0       H+ B(OH)4-            FW86
538     1  .0        .0        .0        .0       H+ B3O3(OH)4-         FW86
539     1  .0        .0        .0        .0       H+ B4O5(OH)4=         FW86
540     1  .0        .0        .0        .0       H+ Br-
541     1  .0        .0        .0        .0       H+ Am(CO3)2-
542     1  .0        .0        .0        .0       H+ Am(CO3)3=-
543     1  .1747     .2931     .0        .00819   H+ ClO4-              P91
544     1  .0        .0        .0        .0       H+ NpO2(OH)2-
545     1  .0        .0        .0        .0       H+ NpO2CO3-
546     1  .0        .0        .0        .0       H+ NpO2(CO3)2=-
547     1  .0        .0        .0        .0       H+ NpO2(CO3)3==-
548     1  .0        .0        .0        .0       H+ H2PO4-
549     1  .0        .0        .0        .0       H+ HPO4=
550     1  .0        .0        .0        .0       H+ PO4=-
551     1  .84       .0        .0        .0       H+ Th(SO4)3=          FR92
552     1  .0        .0        .0        .0       H+ Th(OH)3(CO3)-
553     1  .0        .0        .0        .0       H+ Th(CO3)5===
554     1  .0        .0        .0        .0       H+ HOx-
555     1  .0        .0        .0        .0       H+ Ox=
556     1  .0        .0        .0        .0       H+ Ac-
557     1  .0        .0        .0        .0       H+ Lac-
558     1  .0        .0        .0        .0       H+ H2Cit-
559     1  .0        .0        .0        .0       H+ HCit=
560     1  .0        .0        .0        .0       H+ Cit=-
561     1  .0        .0        .0        .0       H+ H3EDTA-
562     1  .0        .0        .0        .0       H+ H2EDTA=
563     1  .0        .0        .0        .0       H+ HEDTA=-
564     1  .0        .0        .0        .0       H+ EDTA==
565     1  .0        .0        .0        .0       H+ AmEDTA=-
566     1  .0        .0        .0        .0       H+ NpO2Cit=
567     1  .0        .0        .0        .0       H+ NpO2EDTA==-
568     1  .0        .0        .0        .0       H+ NpO2Ox-
569     1  .0        .0        .0        .0       H+ U(OH)4(CO3)2=-
570     1  .0        .0        .0        .0       H+ U(CO3)5===
571     1  .0        .0        .0        .0       H+ U(SO4)3=
572     1  .0        .0        .0        .0       H+ Pu(CO3)2-
573     1  .0        .0        .0        .0       H+ Pu(CO3)3=-
574     1  .0        .0        .0        .0       H+ PuEDTA-
575     1  .0        .0        .0        .0       H+ CaCit-
576     1  .0        .0        .0        .0       H+ CaEDTA=
577     1  .0        .0        .0        .0       H+ UnuAn#2-
578     1  .0        .0        .0        .0       H+ UnuAn#3-
579     1  .0        .0        .0        .0       H+ UnuAn#4-
580     1  .0        .0        .0        .0       H+ U(OH)2(CO3)2=
581     1  .0        .0        .0        .0       H+ MgCit-
582     1  .0        .0        .0        .0       H+ MgEDTA=
583     1  .0        .0        .0        .0       H+ UnuAn#1-
584
585     1  .16       .0        .0        .0       MgB(OH)4+ Cl-         HMW84
586     1  .0        .0        .0        .0       MgB(OH)4+ SO4=        HMW84
587     1  .0        .0        .0        .0       MgB(OH)4+ HSO4-       HMW84
588     1  .0        .0        .0        .0       MgB(OH)4+ OH-         HMW84
589     1  .0        .0        .0        .0       MgB(OH)4+ HCO3-       HMW84
590     1  .0        .0        .0        .0       MgB(OH)4+ CO3=        HMW84
591     1  .0        .0        .0        .0       MgB(OH)4+ B(OH)4-
592     1  .0        .0        .0        .0       MgB(OH)4+ B3O3(OH)4-
593     1  .0        .0        .0        .0       MgB(OH)4+ B4O5(OH)4=
594     1  .0        .0        .0        .0       MgB(OH)4+ Br-
595     1  .0        .0        .0        .0       MgB(OH)4+ Am(CO3)2-
596     1  .0        .0        .0        .0       MgB(OH)4+ Am(CO3)3=-
597     1  .0        .0        .0        .0       MgB(OH)4+ ClO4-
598     1  .0        .0        .0        .0       MgB(OH)4+ NpO2(OH)2-
599     1  .0        .0        .0        .0       MgB(OH)4+ NpO2CO3-
600     1  .0        .0        .0        .0       MgB(OH)4+ NpO2(CO3)2=-
601     1  .0        .0        .0        .0       MgB(OH)4+ NpO2(CO3)3==-
602     1  .0        .0        .0        .0       MgB(OH)4+ H2PO4-
603     1  .0        .0        .0        .0       MgB(OH)4+ HPO4=
604     1  .0        .0        .0        .0       MgB(OH)4+ PO4=-
605     1  .0        .0        .0        .0       MgB(OH)4+ Th(SO4)3=
606     1  .0        .0        .0        .0       MgB(OH)4+ Th(OH)3(CO3)-
607     1  .0        .0        .0        .0       MgB(OH)4+ Th(CO3)5===
608     1  .0        .0        .0        .0       MgB(OH)4+ HOx-
609     1  .0        .0        .0        .0       MgB(OH)4+ Ox=
610     1  .0        .0        .0        .0       MgB(OH)4+ Ac-
611     1  .0        .0        .0        .0       MgB(OH)4+ Lac-
612     1  .0        .0        .0        .0       MgB(OH)4+ H2Cit-
613     1  .0        .0        .0        .0       MgB(OH)4+ HCit=
614     1  .0        .0        .0        .0       MgB(OH)4+ Cit=-
615     1  .0        .0        .0        .0       MgB(OH)4+ H3EDTA-
616     1  .0        .0        .0        .0       MgB(OH)4+ H2EDTA=
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
517     1  .0        .0        .0        .0        MgB(OH)4+ HEDTA=-
518     1  .0        .0        .0        .0        MgB(OH)4+ EDTA==
519     1  .0        .0        .0        .0        MgB(OH)4+ AmEDTA=-
520     1  .0        .0        .0        .0        MgB(OH)4+ NpO2Cit=
521     1  .0        .0        .0        .0        MgB(OH)4+ NpO2EDTA==-
522     1  .0        .0        .0        .0        MgB(OH)4+ NpO2Ox-
523     1  .0        .0        .0        .0        MgB(OH)4+ U(OH)4(CO3)2==
524     1  .0        .0        .0        .0        MgB(OH)4+ U(CO3)5===
525     1  .0        .0        .0        .0        MgB(OH)4+ U(SO4)3=
526     1  .0        .0        .0        .0        MgB(OH)4+ Pu(CO3)2-
527     1  .0        .0        .0        .0        MgB(OH)4+ Pu(CO3)3=-
528     1  .0        .0        .0        .0        MgB(OH)4+ PuEDTA-
529     1  .0        .0        .0        .0        MgB(OH)4+ CaCit-
530     1  .0        .0        .0        .0        MgB(OH)4+ CaEDTA=
531     1  .0        .0        .0        .0        MgB(OH)4+ UmuAn#2-
532     1  .0        .0        .0        .0        MgB(OH)4+ UmuAn#3-
533     1  .0        .0        .0        .0        MgB(OH)4+ UmuAn#4-
534     1  .0        .0        .0        .0        MgB(OH)4+ U(OH)2(CO3)2=
535     1  .0        .0        .0        .0        MgB(OH)4+ MgCit-
536     1  .0        .0        .0        .0        MgB(OH)4+ MgEDTA=
537     1  .0        .0        .0        .0        MgB(OH)4+ UmuAn#1-
538
539     1  .12       .0        .0        .0        CaB(OH)4+ Cl-
540     1  .0        .0        .0        .0        CaB(OH)4+ SO4=      HMW84
541     1  .0        .0        .0        .0        CaB(OH)4+ HSO4-     HMW84
542     1  .0        .0        .0        .0        CaB(OH)4+ OH-       HMW84
543     1  .0        .0        .0        .0        CaB(OH)4+ HCO3-     HMW84
544     1  .0        .0        .0        .0        CaB(OH)4+ CO3=      HMW84
545     1  .0        .0        .0        .0        CaB(OH)4+ B(OH)4-
546     1  .0        .0        .0        .0        CaB(OH)4+ B3O3(OH)4-
547     1  .0        .0        .0        .0        CaB(OH)4+ B4O5(OH)4=
548     1  .0        .0        .0        .0        CaB(OH)4+ Br-
549     1  .0        .0        .0        .0        CaB(OH)4+ Am(CO3)2-
550     1  .0        .0        .0        .0        CaB(OH)4+ Am(CO3)3=-
551     1  .0        .0        .0        .0        CaB(OH)4+ ClO4-
552     1  .0        .0        .0        .0        CaB(OH)4+ NpO2(OH)2-
553     1  .0        .0        .0        .0        CaB(OH)4+ NpO2CO3-
554     1  .0        .0        .0        .0        CaB(OH)4+ NpO2(CO3)2=-
555     1  .0        .0        .0        .0        CaB(OH)4+ NpO2(CO3)3==-
556     1  .0        .0        .0        .0        CaB(OH)4+ H2PO4-
557     1  .0        .0        .0        .0        CaB(OH)4+ HPO4=
558     1  .0        .0        .0        .0        CaB(OH)4+ PO4==
559     1  .0        .0        .0        .0        CaB(OH)4+ Th(SO4)3=
560     1  .0        .0        .0        .0        CaB(OH)4+ Th(OH)3(CO3)-
561     1  .0        .0        .0        .0        CaB(OH)4+ Th(CO3)5===
562     1  .0        .0        .0        .0        CaB(OH)4+ HOx-
563     1  .0        .0        .0        .0        CaB(OH)4+ Ox=
564     1  .0        .0        .0        .0        CaB(OH)4+ Ac-
565     1  .0        .0        .0        .0        CaB(OH)4+ Lac-
566     1  .0        .0        .0        .0        CaB(OH)4+ H2Cit-
567     1  .0        .0        .0        .0        CaB(OH)4+ HCit=
568     1  .0        .0        .0        .0        CaB(OH)4+ Cit=-
569     1  .0        .0        .0        .0        CaB(OH)4+ H3EDTA-
570     1  .0        .0        .0        .0        CaB(OH)4+ H2EDTA=
571     1  .0        .0        .0        .0        CaB(OH)4+ HEDTA=-
572     1  .0        .0        .0        .0        CaB(OH)4+ EDTA==
573     1  .0        .0        .0        .0        CaB(OH)4+ AmEDTA=-
574     1  .0        .0        .0        .0        CaB(OH)4+ NpO2Cit=
575     1  .0        .0        .0        .0        CaB(OH)4+ NpO2EDTA==-
576     1  .0        .0        .0        .0        CaB(OH)4+ NpO2Ox-
577     1  .0        .0        .0        .0        CaB(OH)4+ U(OH)4(CO3)2==
578     1  .0        .0        .0        .0        CaB(OH)4+ U(CO3)5===
579     1  .0        .0        .0        .0        CaB(OH)4+ U(SO4)3=
580     1  .0        .0        .0        .0        CaB(OH)4+ Pu(CO3)2-
581     1  .0        .0        .0        .0        CaB(OH)4+ Pu(CO3)3=-
582     1  .0        .0        .0        .0        CaB(OH)4+ PuEDTA-
583     1  .0        .0        .0        .0        CaB(OH)4+ CaCit-
584     1  .0        .0        .0        .0        CaB(OH)4+ CaEDTA=
585     1  .0        .0        .0        .0        CaB(OH)4+ UmuAn#2-
586     1  .0        .0        .0        .0        CaB(OH)4+ UmuAn#3-
587     1  .0        .0        .0        .0        CaB(OH)4+ UmuAn#4-
588     1  .0        .0        .0        .0        CaB(OH)4+ U(OH)2(CO3)2=
589     1  .0        .0        .0        .0        CaB(OH)4+ MgCit-
590     1  .0        .0        .0        .0        CaB(OH)4+ MgEDTA=
591     1  .0        .0        .0        .0        CaB(OH)4+ UmuAn#1-
592
593     1  .6117     5.403     .0     -0.0284      Am+++ Cl-           FRSR89 (from NdCl3 values)
594     3 3.0398     .0     -2500     .0           Am+++ SO4=          RFP94
595     1  .0        .0        .0        .0        Am+++ HSO4-
596     1  .0        .0        .0        .0        Am+++ OH-
597     1  .0        .0        .0        .0        Am+++ HCO3-
598     3  .0        .0        .0        .0        Am+++ CO3=
599     1  .0        .0        .0        .0        Am+++ B(OH)4-
600     1  .0        .0        .0        .0        Am+++ B3O3(OH)4-
601     3  .0        .0        .0        .0        Am+++ B4O5(OH)4=
602     1  .0        .0        .0        .0        Am+++ Br-
603     1  .0        .0        .0        .0        Am+++ Am(CO3)2-
604     3  .0        .0        .0        .0        Am+++ Am(CO3)3=-
605     1  .80       5.35      .0     -0.0048      Am+++ ClO4-         FRF90
606     1  .0        .0        .0        .0        Am+++ NpO2(OH)2-
607     1  .0        .0        .0        .0        Am+++ NpO2CO3-
608     3  .0        .0        .0        .0        Am+++ NpO2(CO3)2=-
609     3  .0        .0        .0        .0        Am+++ NpO2(CO3)3==-
610     1  .0        .0      -92.9       .0        Am+++ H2PO4-        RFP94 (from Nd-H2PO4 value)
611     3  .0        .0        .0        .0        Am+++ HPO4=
612     3  .0        .0        .0        .0        Am+++ PO4=-
613     3  .0        .0        .0        .0        Am+++ Th(SO4)3=
614     1  .0        .0        .0        .0        Am+++ Th(OH)3(CO3)-
615     3  .0        .0        .0        .0        Am+++ Th(CO3)5===
616     1  .0        .0        .0        .0        Am+++ HOx-
617     3  .0        .0        .0        .0        Am+++ Ox=
618     1  .0        .0        .0        .0        Am+++ Ac-
619     1  .0        .0        .0        .0        Am+++ Lac-
620     1  .0        .0        .0        .0        Am+++ H2Cit-
621     3  .0        .0        .0        .0        Am+++ HCit=
622     3  .0        .0        .0        .0        Am+++ Cit=-
623     3  .0        .0        .0        .0        Am+++ H3EDTA-
624     3  .0        .0        .0        .0        Am+++ H2EDTA=
625     3  .0        .0        .0        .0        Am+++ HEDTA=-
626     3  .0        .0        .0        .0        Am+++ EDTA==
627     3  .0        .0        .0        .0        Am+++ AmEDTA=-
628     3  .0        .0        .0        .0        Am+++ NpO2Cit=
629     3  .0        .0        .0        .0        Am+++ NpO2EDTA==-
630     1  .0        .0        .0        .0        Am+++ NpO2Ox-
631     3  .0        .0        .0        .0        Am+++ U(OH)4(CO3)2==
632     3  .0        .0        .0        .0        Am+++ U(CO3)5===
633     3  .0        .0        .0        .0        Am+++ U(SO4)3=
634     1  .0        .0        .0        .0        Am+++ Pu(CO3)2-
635     3  .0        .0        .0        .0        Am+++ Pu(CO3)3=-
636     1  .0        .0        .0        .0        Am+++ PuEDTA-
637     1  .0        .0        .0        .0        Am+++ CaCit-
638     3  .0        .0        .0        .0        Am+++ CaEDTA=
639     3  .0        .0        .0        .0        Am+++ UmuAn#2-
640     1  .0        .0        .0        .0        Am+++ UmuAn#3-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
741     3  .0        .0        .0        .0       Am+++ UnuAn#4-
742     3  .0        .0        .0        .0       Am+++ U(OH)2(CO3)2=
743     1  .0        .0        .0        .0       Am+++ MgCit-
744     3  .0        .0        .0        .0       Am+++ MgEDTA=
745     1  .0        .0        .0        .0       Am+++ UnuAn#1-
746
747     1  .0        .0        .0        .0       AmCO3+ Cl-
748     1  .0        .0        .0        .0       AmCO3+ SO4=
749     1  .0        .0        .0        .0       AmCO3+ HSO4-
750     1  .0        .0        .0        .0       AmCO3+ OH-
751     1  .0        .0        .0        .0       AmCO3+ HCO3-
752     1  .0        .0        .0        .0       AmCO3+ CO3=
753     1  .0        .0        .0        .0       AmCO3+ B(OH)4-
754     1  .0        .0        .0        .0       AmCO3+ B3O3(OH)4-
755     1  .0        .0        .0        .0       AmCO3+ B4O5(OH)4=
756     1  .0        .0        .0        .0       AmCO3+ Br-
757     1  .0        .0        .0        .0       AmCO3+ Am(CO3)2-
758     1  .0        .0        .0        .0       AmCO3+ Am(CO3)3=-
759     1  .0        .0        .0        .0       AmCO3+ ClO4-
760     1  .0        .0        .0        .0       AmCO3+ NpO2(OH)2-
761     1  .0        .0        .0        .0       AmCO3+ NpO2CO3-
762     1  .0        .0        .0        .0       AmCO3+ NpO2(CO3)2=-
763     1  .0        .0        .0        .0       AmCO3+ NpO2(CO3)3=--
764     1  .0        .0        .0        .0       AmCO3+ H2PO4-
765     1  .0        .0        .0        .0       AmCO3+ HPO4=
766     1  .0        .0        .0        .0       AmCO3+ PO4=-
767     1  .0        .0        .0        .0       AmCO3+ Th(SO4)3=
768     1  .0        .0        .0        .0       AmCO3+ Th(OH)3(CO3)-
769     1  .0        .0        .0        .0       AmCO3+ Th(CO3)5=--
770     1  .0        .0        .0        .0       AmCO3+ HOx-
771     1  .0        .0        .0        .0       AmCO3+ Ox=
772     1  .0        .0        .0        .0       AmCO3+ Ac-
773     1  .0        .0        .0        .0       AmCO3+ Lac-
774     1  .0        .0        .0        .0       AmCO3+ H2Cit-
775     1  .0        .0        .0        .0       AmCO3+ HCit=
776     1  .0        .0        .0        .0       AmCO3+ Cit=-
777     1  .0        .0        .0        .0       AmCO3+ H3EDTA-
778     1  .0        .0        .0        .0       AmCO3+ H2EDTA=
779     1  .0        .0        .0        .0       AmCO3+ HEDTA=-
780     1  .0        .0        .0        .0       AmCO3+ EDTA=-
781     1  .0        .0        .0        .0       AmCO3+ AmEDTA=-
782     1  .0        .0        .0        .0       AmCO3+ NpO2Cit=
783     1  .0        .0        .0        .0       AmCO3+ NpO2EDTA=-
784     1  .0        .0        .0        .0       AmCO3+ NpO2Ox-
785     1  .0        .0        .0        .0       AmCO3+ U(OH)4(CO3)2=
786     1  .0        .0        .0        .0       AmCO3+ U(CO3)5=--
787     1  .0        .0        .0        .0       AmCO3+ U(SO4)3=
788     1  .0        .0        .0        .0       AmCO3+ Pu(CO3)2-
789     1  .0        .0        .0        .0       AmCO3+ Pu(CO3)3=-
790     1  .0        .0        .0        .0       AmCO3+ PuEDTA-
791     1  .0        .0        .0        .0       AmCO3+ CaCit-
792     1  .0        .0        .0        .0       AmCO3+ CaEDTA=
793     1  .0        .0        .0        .0       AmCO3+ UnuAn#2-
794     1  .0        .0        .0        .0       AmCO3+ UnuAn#3-
795     1  .0        .0        .0        .0       AmCO3+ UnuAn#4-
796     1  .0        .0        .0        .0       AmCO3+ U(OH)2(CO3)2=
797     1  .0        .0        .0        .0       AmCO3+ MgCit-
798     1  .0        .0        .0        .0       AmCO3+ MgEDTA=
799     1  .0        .0        .0        .0       AmCO3+ UnuAn#1-
800
801     1 1.092    13.7      -160.      -.112     Th++++ Cl-              Roy92
802     3 1.56        .0        .0        .0     Th++++ SO4=             FR92
803     1 1.44        .0        .0        .0     Th++++ HSO4-            FR92
804     1  .0        .0        .0        .0       Th++++ OH-
805     1  .0        .0        .0        .0       Th++++ HCO3-
806     3  .0        .0        .0        .0       Th++++ CO3=
807     1  .0        .0        .0        .0       Th++++ B(OH)4-
808     1  .0        .0        .0        .0       Th++++ B3O3(OH)4-
809     3  .0        .0        .0        .0       Th++++ B4O5(OH)4=
810     1  .0        .0        .0        .0       Th++++ Br-
811     1  .0        .0        .0        .0       Th++++ Am(CO3)2-
812     3  .0        .0        .0        .0       Th++++ Am(CO3)3=-
813     1 1.19     27.3         .0      -.057     Th++++ ClO4-          CFN960119
814     1  .0        .0        .0        .0       Th++++ NpO2(OH)2-
815     1  .0        .0        .0        .0       Th++++ NpO2CO3-
816     3  .0        .0        .0        .0       Th++++ NpO2(CO3)2=-
817     3  .0        .0        .0        .0       Th++++ NpO2(CO3)3=--
818     2  .0        .0        .0        .0       Th++++ H2PO4-
819     3  .0        .0        .0        .0       Th++++ HPO4=
820     3  .0        .0        .0        .0       Th++++ PO4=-
821     3  .0        .0        .0        .0       Th++++ Th(SO4)3=
822     1  .0        .0        .0        .0       Th++++ Th(OH)3(CO3)-
823     3  .0        .0        .0        .0       Th++++ Th(CO3)5=--
824     2  .0        .0        .0        .0       Th++++ HOx-
825     3  .0        .0        .0        .0       Th++++ Ox=
826     1  .0        .0        .0        .0       Th++++ Ac-
827     1  .0        .0        .0        .0       Th++++ Lac-
828     1  .0        .0        .0        .0       Th++++ H2Cit-
829     1  .0        .0        .0        .0       Th++++ HCit=
830     3  .0        .0        .0        .0       Th++++ Cit=-
831     3  .0        .0        .0        .0       Th++++ H3EDTA-
832     3  .0        .0        .0        .0       Th++++ H2EDTA=
833     3  .0        .0        .0        .0       Th++++ HEDTA=-
834     3  .0        .0        .0        .0       Th++++ EDTA=-
835     3  .0        .0        .0        .0       Th++++ AmEDTA=-
836     3  .0        .0        .0        .0       Th++++ NpO2Cit=
837     3  .0        .0        .0        .0       Th++++ NpO2EDTA=-
838     1  .0        .0        .0        .0       Th++++ NpO2Ox-
839     3  .0        .0        .0        .0       Th++++ U(OH)4(CO3)2=
840     3  .0        .0        .0        .0       Th++++ U(CO3)5=--
841     3  .0        .0        .0        .0       Th++++ U(SO4)3=
842     1  .0        .0        .0        .0       Th++++ Pu(CO3)2-
843     3  .0        .0        .0        .0       Th++++ Pu(CO3)3=-
844     1  .0        .0        .0        .0       Th++++ PuEDTA-
845     1  .0        .0        .0        .0       Th++++ CaCit-
846     3  .0        .0        .0        .0       Th++++ CaEDTA=
847     3  .0        .0        .0        .0       Th++++ UnuAn#2-
848     1  .0        .0        .0        .0       Th++++ UnuAn#3-
849     3  .0        .0        .0        .0       Th++++ UnuAn#4-
850     3  .0        .0        .0        .0       Th++++ U(OH)2(CO3)2=
851     1  .0        .0        .0        .0       Th++++ MgCit-
852     3  .0        .0        .0        .0       Th++++ MgEDTA=
853     1  .0        .0        .0        .0       Th++++ UnuAn#1-
854
855     1  .6117    5.403      .0      -0.0284    Pu+++ Cl-          FRSH89 (from NdCl3 values)
856     3 3.0398      .0     -2500        .0      Pu+++ SO4=         RF794
857     1  .0        .0        .0        .0       Pu+++ HSO4-
858     1  .0        .0        .0        .0       Pu+++ OH-
859     1  .0        .0        .0        .0       Pu+++ HCO3-
860     3  .0        .0        .0        .0       Pu+++ CO3=
861     1  .0        .0        .0        .0       Pu+++ B(OH)4-
862     1  .0        .0        .0        .0       Pu+++ B3O3(OH)4-
863     3  .0        .0        .0        .0       Pu+++ B4O5(OH)4=
864     1  .0        .0        .0        .0       Pu+++ Br-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
865     1  .0        .0        .0        .0        Pu+++ Pu(CO3)2-
866     3  .0        .0        .0        .0        Pu+++ Pu(CO3)3=-
867     1  .80      5.35        .0   -0.0048        Pu+++ ClO4-              FRF90
868     1  .0        .0        .0        .0        Pu+++ NpO2(OH)2-
869     1  .0        .0        .0        .0        Pu+++ NpO2CO3-
870     1  .0        .0        .0        .0        Pu+++ NpO2(CO3)2=-
871     3  .0        .0        .0        .0        Pu+++ NpO2(CO3)3===
872     1  .0        .0     -92.5        .0        Pu+++ H2PO4-             RFF96 (from Nd-H2PO4 value)
873     3  .0        .0        .0        .0        Pu+++ HPO4=
874     3  .0        .0        .0        .0        Pu+++ PO4==-
875     3  .0        .0        .0        .0        Pu+++ Th(SO4)3=
876     1  .0        .0        .0        .0        Pu+++ Th(OH)3(CO3)-
877     3  .0        .0        .0        .0        Pu+++ Th(CO3)5===
878     1  .0        .0        .0        .0        Pu+++ HOx-
879     3  .0        .0        .0        .0        Pu+++ Ox=
880     1  .0        .0        .0        .0        Pu+++ Ac-
881     1  .0        .0        .0        .0        Pu+++ Lac-
882     1  .0        .0        .0        .0        Pu+++ H2Cit-
883     3  .0        .0        .0        .0        Pu+++ HCit=
884     3  .0        .0        .0        .0        Pu+++ Cit=-
885     3  .0        .0        .0        .0        Pu+++ H3EDTA-
886     3  .0        .0        .0        .0        Pu+++ H2EDTA=
887     3  .0        .0        .0        .0        Pu+++ HEDTA==-
888     3  .0        .0        .0        .0        Pu+++ EDTA===
889     3  .0        .0        .0        .0        Pu+++ PuEDTA=-
890     3  .0        .0        .0        .0        Pu+++ NpO2Cit=
891     3  .0        .0        .0        .0        Pu+++ NpO2EDTA==-
892     1  .0        .0        .0        .0        Pu+++ NpO2Ox-
893     3  .0        .0        .0        .0        Pu+++ U(OH)4(CO3)2==
894     3  .0        .0        .0        .0        Pu+++ U(CO3)5===
895     3  .0        .0        .0        .0        Pu+++ U(SO4)3=
896     1  .0        .0        .0        .0        Pu+++ Pu(CO3)2-
897     3  .0        .0        .0        .0        Pu+++ Pu(CO3)3=-
898     1  .0        .0        .0        .0        Pu+++ PuEDTA-
899     1  .0        .0        .0        .0        Pu+++ CaCit-
900     3  .0        .0        .0        .0        Pu+++ CaEDTA=
901     3  .0        .0        .0        .0        Pu+++ UnuAn#2-
902     1  .0        .0        .0        .0        Pu+++ UnuAn#3-
903     3  .0        .0        .0        .0        Pu+++ UnuAn#4-
904     3  .0        .0        .0        .0        Pu+++ U(OH)2(CO3)2=
905     1  .0        .0        .0        .0        Pu+++ MgCit-
906     3  .0        .0        .0        .0        Pu+++ MgEDTA=
907     1  .0        .0        .0        .0        Pu+++ UnuAn#1-
908
909     1  .1415     .281        .0        .0        NpO2+ Cl-              NFRK95
910     1  .0        .0        .0        .0        NpO2+ SO4=
911     1  .0        .0        .0        .0        NpO2+ HSO4-
912     1  .0        .0        .0        .0        NpO2+ OH-
913     1  .0        .0        .0        .0        NpO2+ HCO3-
914     1  .0        .0        .0        .0        NpO2+ CO3=
915     1  .0        .0        .0        .0        NpO2+ B(OH)4-
916     1  .0        .0        .0        .0        NpO2+ B3O3(OH)4-
917     1  .0        .0        .0        .0        NpO2+ B4O5(OH)4=
918     1  .0        .0        .0        .0        NpO2+ Br-
919     1  .0        .0        .0        .0        NpO2+ Am(CO3)2-
920     1  .0        .0        .0        .0        NpO2+ Am(CO3)3=-
921     1  .257      .180        .0      .0081       NpO2+ ClO4-              NFRK95
922     1  .0        .0        .0        .0        NpO2+ NpO2(OH)2-
923     1  .0        .0        .0        .0        NpO2+ NpO2CO3-
924     1  .0        .0        .0        .0        NpO2+ NpO2(CO3)2=-
925     1  .0        .0        .0        .0        NpO2+ NpO2(CO3)3===
926     1  .0        .0        .0        .0        NpO2+ H2PO4-
927     1  .0        .0        .0        .0        NpO2+ HPO4=
928     1  .0        .0        .0        .0        NpO2+ PO4==-
929     1  .0        .0        .0        .0        NpO2+ Th(SO4)3=
930     1  .0        .0        .0        .0        NpO2+ Th(OH)3(CO3)-
931     1  .0        .0        .0        .0        NpO2+ Th(CO3)5===
932     1  .0        .0        .0        .0        NpO2+ HOx-
933     1  .0        .0        .0        .0        NpO2+ Ox=
934     1  .0        .0        .0        .0        NpO2+ Ac-
935     1  .0        .0        .0        .0        NpO2+ Lac-
936     1  .0        .0        .0        .0        NpO2+ H2Cit-
937     1  .0        .0        .0        .0        NpO2+ HCit=
938     1  .0        .0        .0        .0        NpO2+ Cit=-
939     1  .0        .0        .0        .0        NpO2+ H3EDTA-
940     1  .0        .0        .0        .0        NpO2+ H2EDTA=
941     1  .0        .0        .0        .0        NpO2+ HEDTA==-
942     1  .0        .0        .0        .0        NpO2+ EDTA===
943     1  .0        .0        .0        .0        NpO2+ AmEDTA=-
944     1  .0        .0        .0        .0        NpO2+ NpO2Cit=
945     1  .0        .0        .0        .0        NpO2+ NpO2EDTA==-
946     1  .0        .0        .0        .0        NpO2+ NpO2Ox-
947     1  .0        .0        .0        .0        NpO2+ U(OH)4(CO3)2==
948     1  .0        .0        .0        .0        NpO2+ U(CO3)5===
949     1  .0        .0        .0        .0        NpO2+ U(SO4)3=
950     1  .0        .0        .0        .0        NpO2+ Pu(CO3)2-
951     1  .0        .0        .0        .0        NpO2+ Pu(CO3)3=-
952     1  .0        .0        .0        .0        NpO2+ PuEDTA-
953     1  .0        .0        .0        .0        NpO2+ CaCit-
954     1  .0        .0        .0        .0        NpO2+ CaEDTA=
955     1  .0        .0        .0        .0        NpO2+ UnuAn#2-
956     1  .0        .0        .0        .0        NpO2+ UnuAn#3-
957     1  .0        .0        .0        .0        NpO2+ UnuAn#4-
958     1  .0        .0        .0        .0        NpO2+ U(OH)2(CO3)2=
959     1  .0        .0        .0        .0        NpO2+ MgCit-
960     1  .0        .0        .0        .0        NpO2+ MgEDTA=
961     1  .0        .0        .0        .0        NpO2+ UnuAn#1-
962
963     1 1.644    15.5        .0        .1        U++++ Cl-              RFSM90
964     3  .0        .0        .0        .0        U++++ SO4=
965     1  .0        .0        .0        .0        U++++ HSO4-
966     1  .0        .0        .0        .0        U++++ OH-
967     1  .0        .0        .0        .0        U++++ HCO3-
968     3  .0        .0        .0        .0        U++++ CO3=
969     1  .0        .0        .0        .0        U++++ B(OH)4-
970     1  .0        .0        .0        .0        U++++ B3O3(OH)4-
971     3  .0        .0        .0        .0        U++++ B4O5(OH)4=
972     1  .0        .0        .0        .0        U++++ Br-
973     1  .0        .0        .0        .0        U++++ Am(CO3)2-
974     3  .0        .0        .0        .0        U++++ Am(CO3)3=-
975     1  .0        .0        .0        .0        U++++ ClO4-
976     1  .0        .0        .0        .0        U++++ NpO2(OH)2-
977     1  .0        .0        .0        .0        U++++ NpO2CO3-
978     3  .0        .0        .0        .0        U++++ NpO2(CO3)2=-
979     3  .0        .0        .0        .0        U++++ NpO2(CO3)3===
980     1  .0        .0        .0        .0        U++++ H2PO4-
981     3  .0        .0        .0        .0        U++++ HPO4=
982     3  .0        .0        .0        .0        U++++ PO4==-
983     3  .0        .0        .0        .0        U++++ Th(SO4)3=
984     1  .0        .0        .0        .0        U++++ Th(OH)3(CO3)-
985     3  .0        .0        .0        .0        U++++ Th(CO3)5===
986     1  .0        .0        .0        .0        U++++ HOx-
987     3  .0        .0        .0        .0        U++++ Ox=
988     1  .0        .0        .0        .0        U++++ Ac-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
989     1  .0        .0        .0        .0      U++++ Lac-
990     1  .0        .0        .0        .0      U++++ H2Cit-
991     3  .0        .0        .0        .0      U++++ HCit=
992     3  .0        .0        .0        .0      U++++ Cit=-
993     3  .0        .0        .0        .0      U++++ H3EDTA-
994     3  .0        .0        .0        .0      U++++ H2EDTA=
995     3  .0        .0        .0        .0      U++++ HEDTA=-
996     3  .0        .0        .0        .0      U++++ EDTA==
997     3  .0        .0        .0        .0      U++++ AmEDTA=-
998     3  .0        .0        .0        .0      U++++ NpO2Cit=
999     3  .0        .0        .0        .0      U++++ NpO2EDTA==-
1000    1  .0        .0        .0        .0      U++++ NpO2Ox-
1001    3  .0        .0        .0        .0      U++++ U(OH)4(CO3)2==
1002    3  .0        .0        .0        .0      U++++ U(CO3)5===
1003    3  .0        .0        .0        .0      U++++ U(SO4)3=
1004    1  .0        .0        .0        .0      U++++ Pu(CO3)2-
1005    3  .0        .0        .0        .0      U++++ Pu(CO3)3=-
1006    1  .0        .0        .0        .0      U++++ PuEDTA-
1007    1  .0        .0        .0        .0      U++++ CaCit-
1008    3  .0        .0        .0        .0      U++++ CaEDTA=
1009    3  .0        .0        .0        .0      U++++ UnuAn#2-
1010    1  .0        .0        .0        .0      U++++ UnuAn#3-
1011    3  .0        .0        .0        .0      U++++ UnuAn#4-
1012    3  .0        .0        .0        .0      U++++ U(OH)2(CO3)2=
1013    1  .0        .0        .0        .0      U++++ MgCit-
1014    3  .0        .0        .0        .0      U++++ MgEDTA=
1015    1  .0        .0        .0        .0      U++++ UnuAn#1-
1016
1017    1 1.0       7.856      .0        .0      UOH+++ Cl-          RF#2005
1018    3  .0        .0        .0        .0      UOH+++ SO4=
1019    1  .0        .0        .0        .0      UOH+++ HSO4-
1020    1  .0        .0        .0        .0      UOH+++ OH-
1021    1  .0        .0        .0        .0      UOH+++ HCO3-
1022    3  .0        .0        .0        .0      UOH+++ CO3=
1023    1  .0        .0        .0        .0      UOH+++ B(OH)4-
1024    1  .0        .0        .0        .0      UOH+++ B3O3(OH)4-
1025    3  .0        .0        .0        .0      UOH+++ B4O5(OH)4=
1026    1  .0        .0        .0        .0      UOH+++ Br-
1027    1  .0        .0        .0        .0      UOH+++ Am(CO3)2-
1028    3  .0        .0        .0        .0      UOH+++ Am(CO3)3=-
1029    1  .0        .0        .0        .0      UOH+++ ClO4-
1030    1  .0        .0        .0        .0      UOH+++ NpO2(OH)2-
1031    1  .0        .0        .0        .0      UOH+++ NpO2CO3-
1032    3  .0        .0        .0        .0      UOH+++ NpO2(CO3)2=-
1033    3  .0        .0        .0        .0      UOH+++ NpO2(CO3)3==-
1034    1  .0        .0        .0        .0      UOH+++ H2PO4-
1035    3  .0        .0        .0        .0      UOH+++ HPO4=
1036    3  .0        .0        .0        .0      UOH+++ PO4=-
1037    3  .0        .0        .0        .0      UOH+++ Th(SO4)3=
1038    1  .0        .0        .0        .0      UOH+++ Th(OH)3(CO3)-
1039    3  .0        .0        .0        .0      UOH+++ Th(CO3)5===
1040    1  .0        .0        .0        .0      UOH+++ HOx-
1041    3  .0        .0        .0        .0      UOH+++ Ox=
1042    1  .0        .0        .0        .0      UOH+++ Ac-
1043    1  .0        .0        .0        .0      UOH+++ Lac-
1044    1  .0        .0        .0        .0      UOH+++ H2Cit-
1045    3  .0        .0        .0        .0      UOH+++ HCit=
1046    3  .0        .0        .0        .0      UOH+++ Cit=-
1047    3  .0        .0        .0        .0      UOH+++ H3EDTA-
1048    3  .0        .0        .0        .0      UOH+++ H2EDTA=
1049    3  .0        .0        .0        .0      UOH+++ HEDTA=-
1050    3  .0        .0        .0        .0      UOH+++ EDTA==
1051    3  .0        .0        .0        .0      UOH+++ AmEDTA=-
1052    3  .0        .0        .0        .0      UOH+++ NpO2Cit=
1053    3  .0        .0        .0        .0      UOH+++ NpO2EDTA==-
1054    1  .0        .0        .0        .0      UOH+++ NpO2Ox-
1055    3  .0        .0        .0        .0      UOH+++ U(OH)4(CO3)2==
1056    3  .0        .0        .0        .0      UOH+++ U(CO3)5===
1057    3  .0        .0        .0        .0      UOH+++ U(SO4)3=
1058    1  .0        .0        .0        .0      UOH+++ Pu(CO3)2-
1059    3  .0        .0        .0        .0      UOH+++ Pu(CO3)3=-
1060    1  .0        .0        .0        .0      UOH+++ PuEDTA-
1061    1  .0        .0        .0        .0      UOH+++ CaCit-
1062    3  .0        .0        .0        .0      UOH+++ CaEDTA=
1063    3  .0        .0        .0        .0      UOH+++ UnuAn#2-
1064    1  .0        .0        .0        .0      UOH+++ UnuAn#3-
1065    3  .0        .0        .0        .0      UOH+++ UnuAn#4-
1066    3  .0        .0        .0        .0      UOH+++ U(OH)2(CO3)2=
1067    1  .0        .0        .0        .0      UOH+++ MgCit-
1068    3  .0        .0        .0        .0      UOH+++ MgEDTA=
1069    1  .0        .0        .0        .0      UOH+++ UnuAn#1-
1070
1071    1 1.239     6.934      .0        .0      UAc+++ Cl-        analogy w/ThAc+++
1072    3  .0        .0        .0        .0      UAc+++ SO4=
1073    1  .0        .0        .0        .0      UAc+++ HSO4-
1074    1  .0        .0        .0        .0      UAc+++ OH-
1075    1  .0        .0        .0        .0      UAc+++ HCO3-
1076    3  .0        .0        .0        .0      UAc+++ CO3=
1077    1  .0        .0        .0        .0      UAc+++ B(OH)4-
1078    1  .0        .0        .0        .0      UAc+++ B3O3(OH)4-
1079    3  .0        .0        .0        .0      UAc+++ B4O5(OH)4=
1080    1  .0        .0        .0        .0      UAc+++ Br-
1081    1  .0        .0        .0        .0      UAc+++ Am(CO3)2-
1082    3  .0        .0        .0        .0      UAc+++ Am(CO3)3=-
1083    1  .0        .0        .0        .0      UAc+++ ClO4-
1084    1  .0        .0        .0        .0      UAc+++ NpO2(OH)2-
1085    1  .0        .0        .0        .0      UAc+++ NpO2CO3-
1086    3  .0        .0        .0        .0      UAc+++ NpO2(CO3)2=-
1087    3  .0        .0        .0        .0      UAc+++ NpO2(CO3)3==-
1088    1  .0        .0        .0        .0      UAc+++ H2PO4-
1089    3  .0        .0        .0        .0      UAc+++ HPO4=
1090    3  .0        .0        .0        .0      UAc+++ PO4=-
1091    3  .0        .0        .0        .0      UAc+++ Th(SO4)3=
1092    1  .0        .0        .0        .0      UAc+++ Th(OH)3(CO3)-
1093    3  .0        .0        .0        .0      UAc+++ Th(CO3)5===
1094    1  .0        .0        .0        .0      UAc+++ HOx-
1095    1  .0        .0        .0        .0      UAc+++ Ox=
1096    1  .0        .0        .0        .0      UAc+++ Ac-
1097    1  .0        .0        .0        .0      UAc+++ Lac-
1098    1  .0        .0        .0        .0      UAc+++ H2Cit-
1099    3  .0        .0        .0        .0      UAc+++ HCit=
1100    3  .0        .0        .0        .0      UAc+++ Cit=-
1101    3  .0        .0        .0        .0      UAc+++ H3EDTA-
1102    3  .0        .0        .0        .0      UAc+++ H2EDTA=
1103    3  .0        .0        .0        .0      UAc+++ HEDTA=-
1104    3  .0        .0        .0        .0      UAc+++ EDTA==
1105    3  .0        .0        .0        .0      UAc+++ AmEDTA=-
1106    3  .0        .0        .0        .0      UAc+++ NpO2Cit=
1107    3  .0        .0        .0        .0      UAc+++ NpO2EDTA==-
1108    1  .0        .0        .0        .0      UAc+++ NpO2Ox-
1109    3  .0        .0        .0        .0      UAc+++ U(OH)4(CO3)2==
1110    3  .0        .0        .0        .0      UAc+++ U(CO3)5===
1111    3  .0        .0        .0        .0      UAc+++ U(SO4)3=
1112    1  .0        .0        .0        .0      UAc+++ Pu(CO3)2-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
1113    3  .0        .0        .0        .0      UAc+++ Pu(CO3)3-
1114    1  .0        .0        .0        .0      UAc+++ PuEDTA-
1115    1  .0        .0        .0        .0      UAc+++ CaCit-
1116    3  .0        .0        .0        .0      UAc+++ CaEDTA=
1117    3  .0        .0        .0        .0      UAc+++ UnuAn#2-
1118    1  .0        .0        .0        .0      UAc+++ UnuAn#3-
1119    3  .0        .0        .0        .0      UAc+++ UnuAn#4-
1120    3  .0        .0        .0        .0      UAc+++ U(OH)2(CO3)2=
1121    1  .0        .0        .0        .0      UAc+++ MgCit-
1122    3  .0        .0        .0        .0      UAc+++ MgEDTA=
1123    1  .0        .0        .0        .0      UAc+++ UnuAn#1-
1124
1125    1 -.2061    -.525      .0        .0      ThOx++ Cl-              RCH96
1126    2  .0        .0        .0        .0      ThOx++ SO4=
1127    1  .0        .0        .0        .0      ThOx++ HSO4-
1128    1  .0        .0        .0        .0      ThOx++ OH-
1129    1  .0        .0        .0        .0      ThOx++ HCO3-
1130    2  .0        .0        .0        .0      ThOx++ CO3=
1131    1  .0        .0        .0        .0      ThOx++ B(OH)4-
1132    1  .0        .0        .0        .0      ThOx++ BJO3(OH)4-
1133    2  .0        .0        .0        .0      ThOx++ B4O5(OH)4=
1134    1  .0        .0        .0        .0      ThOx++ Br-
1135    1  .0        .0        .0        .0      ThOx++ Am(CO3)2-
1136    3  .0        .0        .0        .0      ThOx++ Am(CO3)3=
1137    1  .0        .0        .0        .0      ThOx++ ClO4-
1138    1  .0        .0        .0        .0      ThOx++ NpO2(OH)2-
1139    1  .0        .0        .0        .0      ThOx++ NpO2CO3-
1140    2  .0        .0        .0        .0      ThOx++ NpO2(CO3)2=
1141    3  .0        .0        .0        .0      ThOx++ NpO2(CO3)3==
1142    1  .0        .0        .0        .0      ThOx++ H2PO4-
1143    2  .0        .0        .0        .0      ThOx++ HPO4=
1144    3  .0        .0        .0        .0      ThOx++ PO4=-
1145    2  .0        .0        .0        .0      ThOx++ Th(SO4)3=
1146    1  .0        .0        .0        .0      ThOx++ Th(OH)3(CO3)-
1147    3  .0        .0        .0        .0      ThOx++ Th(CO3)5===
1148    1  .0        .0        .0        .0      ThOx++ HOx-
1149    2  .0        .0        .0        .0      ThOx++ Ox=
1150    1  .0        .0        .0        .0      ThOx++ Ac-
1151    1  .0        .0        .0        .0      ThOx++ Lac-
1152    1  .0        .0        .0        .0      ThOx++ H2Cit-
1153    2  .0        .0        .0        .0      ThOx++ HCit=
1154    3  .0        .0        .0        .0      ThOx++ Cit=-
1155    3  .0        .0        .0        .0      ThOx++ H3EDTA-
1156    3  .0        .0        .0        .0      ThOx++ H2EDTA=
1157    3  .0        .0        .0        .0      ThOx++ HEDTA=-
1158    3  .0        .0        .0        .0      ThOx++ EDTA===
1159    3  .0        .0        .0        .0      ThOx++ AmEDTA=-
1160    2  .0        .0        .0        .0      ThOx++ NpO2Cit=
1161    3  .0        .0        .0        .0      ThOx++ NpO2EDTA==-
1162    1  .0        .0        .0        .0      ThOx++ NpO2Ox-
1163    3  .0        .0        .0        .0      ThOx++ U(OH)4(CO3)2==
1164    3  .0        .0        .0        .0      ThOx++ U(CO3)5===
1165    2  .0        .0        .0        .0      ThOx++ U(SO4)3=
1166    1  .0        .0        .0        .0      ThOx++ Pu(CO3)2-
1167    2  .0        .0        .0        .0      ThOx++ Pu(CO3)3=-
1168    1  .0        .0        .0        .0      ThOx++ PuEDTA-
1169    1  .0        .0        .0        .0      ThOx++ CaCit-
1170    2  .0        .0        .0        .0      ThOx++ CaEDTA=
1171    3  .0        .0        .0        .0      ThOx++ UnuAn#2-
1172    1  .0        .0        .0        .0      ThOx++ UnuAn#3-
1173    2  .0        .0        .0        .0      ThOx++ UnuAn#4-
1174    2  .0        .0        .0        .0      ThOx++ U(OH)2(CO3)2=
1175    1  .0        .0        .0        .0      ThOx++ MgCit-
1176    2  .0        .0        .0        .0      ThOx++ MgEDTA=
1177    1  .0        .0        .0        .0      ThOx++ UnuAn#1-
1178
1179    1  .227     2.154      .0       -.102    AmAc++ Cl-              RCH96
1180    2  .0        .0        .0        .0      AmAc++ SO4=
1181    1  .0        .0        .0        .0      AmAc++ HSO4-
1182    1  .0        .0        .0        .0      AmAc++ OH-
1183    1  .0        .0        .0        .0      AmAc++ HCO3-
1184    2  .0        .0        .0        .0      AmAc++ CO3=
1185    1  .0        .0        .0        .0      AmAc++ B(OH)4-
1186    1  .0        .0        .0        .0      AmAc++ BJO3(OH)4-
1187    2  .0        .0        .0        .0      AmAc++ B4O5(OH)4=
1188    1  .0        .0        .0        .0      AmAc++ Br-
1189    1  .0        .0        .0        .0      AmAc++ Am(CO3)2-
1190    3  .0        .0        .0        .0      AmAc++ Am(CO3)3=
1191    1  .0        .0        .0        .0      AmAc++ ClO4-
1192    1  .0        .0        .0        .0      AmAc++ NpO2(OH)2-
1193    1  .0        .0        .0        .0      AmAc++ NpO2CO3-
1194    2  .0        .0        .0        .0      AmAc++ NpO2(CO3)2=
1195    3  .0        .0        .0        .0      AmAc++ NpO2(CO3)3==
1196    1  .0        .0        .0        .0      AmAc++ H2PO4-
1197    2  .0        .0        .0        .0      AmAc++ HPO4=
1198    3  .0        .0        .0        .0      AmAc++ PO4=-
1199    2  .0        .0        .0        .0      AmAc++ Th(SO4)3=
1200    1  .0        .0        .0        .0      AmAc++ Th(OH)3(CO3)-
1201    3  .0        .0        .0        .0      AmAc++ Th(CO3)5===
1202    1  .0        .0        .0        .0      AmAc++ HOx-
1203    2  .0        .0        .0        .0      AmAc++ Ox=
1204    1  .0        .0        .0        .0      AmAc++ Ac-
1205    1  .0        .0        .0        .0      AmAc++ Lac-
1206    1  .0        .0        .0        .0      AmAc++ H2Cit-
1207    2  .0        .0        .0        .0      AmAc++ HCit=
1208    3  .0        .0        .0        .0      AmAc++ Cit=-
1209    3  .0        .0        .0        .0      AmAc++ H3EDTA-
1210    3  .0        .0        .0        .0      AmAc++ H2EDTA=
1211    3  .0        .0        .0        .0      AmAc++ HEDTA=-
1212    3  .0        .0        .0        .0      AmAc++ EDTA===
1213    3  .0        .0        .0        .0      AmAc++ AmEDTA=-
1214    2  .0        .0        .0        .0      AmAc++ NpO2Cit=
1215    3  .0        .0        .0        .0      AmAc++ NpO2EDTA==-
1216    1  .0        .0        .0        .0      AmAc++ NpO2Ox-
1217    3  .0        .0        .0        .0      AmAc++ U(OH)4(CO3)2==
1218    3  .0        .0        .0        .0      AmAc++ U(CO3)5===
1219    2  .0        .0        .0        .0      AmAc++ U(SO4)3=
1220    1  .0        .0        .0        .0      AmAc++ Pu(CO3)2-
1221    2  .0        .0        .0        .0      AmAc++ Pu(CO3)3=-
1222    1  .0        .0        .0        .0      AmAc++ PuEDTA-
1223    1  .0        .0        .0        .0      AmAc++ CaCit-
1224    2  .0        .0        .0        .0      AmAc++ CaEDTA=
1225    3  .0        .0        .0        .0      AmAc++ UnuAn#2-
1226    1  .0        .0        .0        .0      AmAc++ UnuAn#3-
1227    2  .0        .0        .0        .0      AmAc++ UnuAn#4-
1228    2  .0        .0        .0        .0      AmAc++ U(OH)2(CO3)2=
1229    1  .0        .0        .0        .0      AmAc++ MgCit-
1230    2  .0        .0        .0        .0      AmAc++ MgEDTA=
1231    1  .0        .0        .0        .0      AmAc++ UnuAn#1-
1232
1233    1 -.0572    6.331      .0        .0      AmLac++ Cl-             RCH96
1234    2  .0        .0        .0        .0      AmLac++ SO4=
1235    1  .0        .0        .0        .0      AmLac++ HSO4-
1236    1  .0        .0        .0        .0      AmLac++ OH-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
1237      1  .0        .0        .0        .0       AmLac++ HCO3-
1238      2  .0        .0        .0        .0       AmLac++ CO3=
1239      1  .0        .0        .0        .0       AmLac++ B(OH)4-
1240      1  .0        .0        .0        .0       AmLac++ B3O3(OH)4-
1241      2  .0        .0        .0        .0       AmLac++ B4O5(OH)4=
1242      1  .0        .0        .0        .0       AmLac++ Br-
1243      1  .0        .0        .0        .0       AmLac++ Am(CO3)2-
1244      3  .0        .0        .0        .0       AmLac++ Am(CO3)3=-
1245      1  .0        .0        .0        .0       AmLac++ ClO4-
1246      1  .0        .0        .0        .0       AmLac++ NpO2(OH)2-
1247      1  .0        .0        .0        .0       AmLac++ NpO2CO3-
1248      3  .0        .0        .0        .0       AmLac++ NpO2(CO3)2=-
1249      3  .0        .0        .0        .0       AmLac++ NpO2(CO3)3=-=
1250      1  .0        .0        .0        .0       AmLac++ H2PO4-
1251      2  .0        .0        .0        .0       AmLac++ HPO4=
1252      3  .0        .0        .0        .0       AmLac++ PO4=-
1253      2  .0        .0        .0        .0       AmLac++ Th(SO4)3=
1254      1  .0        .0        .0        .0       AmLac++ Th(OH)3(CO3)-
1255      3  .0        .0        .0        .0       AmLac++ Th(CO3)5=-=
1256      1  .0        .0        .0        .0       AmLac++ HOx-
1257      2  .0        .0        .0        .0       AmLac++ Ox=
1258      1  .0        .0        .0        .0       AmLac++ Ac-
1259      1  .0        .0        .0        .0       AmLac++ Lac-
1260      1  .0        .0        .0        .0       AmLac++ H2Cit-
1261      2  .0        .0        .0        .0       AmLac++ HCit=
1262      3  .0        .0        .0        .0       AmLac++ Cit=-
1263      3  .0        .0        .0        .0       AmLac++ H3EDTA-
1264      3  .0        .0        .0        .0       AmLac++ H2EDTA=
1265      3  .0        .0        .0        .0       AmLac++ HEDTA=-
1266      3  .0        .0        .0        .0       AmLac++ EDTA=-
1267      3  .0        .0        .0        .0       AmLac++ AmEDTA=-
1268      2  .0        .0        .0        .0       AmLac++ NpO2Cit=
1269      3  .0        .0        .0        .0       AmLac++ NpO2EDTA=-
1270      1  .0        .0        .0        .0       AmLac++ NpO2Ox-
1271      3  .0        .0        .0        .0       AmLac++ U(OH)4(CO3)2=-
1272      3  .0        .0        .0        .0       AmLac++ U(CO3)5=-=
1273      2  .0        .0        .0        .0       AmLac++ U(SO4)3=
1274      1  .0        .0        .0        .0       AmLac++ Pu(CO3)2-
1275      2  .0        .0        .0        .0       AmLac++ Pu(CO3)3=-
1276      1  .0        .0        .0        .0       AmLac++ PuEDTA-
1277      1  .0        .0        .0        .0       AmLac++ CaCit-
1278      2  .0        .0        .0        .0       AmLac++ CaEDTA=
1279      3  .0        .0        .0        .0       AmLac++ UnuAn#2-
1280      1  .0        .0        .0        .0       AmLac++ UnuAn#3-
1281      2  .0        .0        .0        .0       AmLac++ UnuAn#4=
1282      2  .0        .0        .0        .0       AmLac++ U(OH)2(CO3)2=
1283      1  .0        .0        .0        .0       AmLac++ MgCit-
1284      2  .0        .0        .0        .0       AmLac++ MgEDTA=
1285      1  .0        .0        .0        .0       AmLac++ UnuAn#1-
1286
1287      1 -.3219     .0        .0        .0       AmOx+ Cl-                RCM96
1288      1  .0        .0        .0        .0       AmOx+ SO4=
1289      1  .0        .0        .0        .0       AmOx+ HSO4-
1290      1  .0        .0        .0        .0       AmOx+ OH-
1291      1  .0        .0        .0        .0       AmOx+ HCO3-
1292      1  .0        .0        .0        .0       AmOx+ CO3=
1293      1  .0        .0        .0        .0       AmOx+ B(OH)4-
1294      1  .0        .0        .0        .0       AmOx+ B3O3(OH)4-
1295      2  .0        .0        .0        .0       AmOx+ B4O5(OH)4=
1296      1  .0        .0        .0        .0       AmOx+ Br-
1297      1  .0        .0        .0        .0       AmOx+ Am(CO3)2-
1298      1  .0        .0        .0        .0       AmOx+ Am(CO3)3=-
1299      1  .0        .0        .0        .0       AmOx+ ClO4-
1300      1  .0        .0        .0        .0       AmOx+ NpO2(OH)2-
1301      1  .0        .0        .0        .0       AmOx+ NpO2CO3-
1302      1  .0        .0        .0        .0       AmOx+ NpO2(CO3)2=-
1303      1  .0        .0        .0        .0       AmOx+ NpO2(CO3)3=-=
1304      1  .0        .0        .0        .0       AmOx+ H2PO4-
1305      1  .0        .0        .0        .0       AmOx+ HPO4=
1306      1  .0        .0        .0        .0       AmOx+ PO4=-
1307      1  .0        .0        .0        .0       AmOx+ Th(SO4)3=
1308      1  .0        .0        .0        .0       AmOx+ Th(OH)3(CO3)-
1309      1  .0        .0        .0        .0       AmOx+ Th(CO3)5=-=
1310      1  .0        .0        .0        .0       AmOx+ HOx-
1311      1  .0        .0        .0        .0       AmOx+ Ox=
1312      1  .0        .0        .0        .0       AmOx+ Ac-
1313      1  .0        .0        .0        .0       AmOx+ Lac-
1314      1  .0        .0        .0        .0       AmOx+ H2Cit-
1315      1  .0        .0        .0        .0       AmOx+ HCit=
1316      1  .0        .0        .0        .0       AmOx+ Cit=-
1317      1  .0        .0        .0        .0       AmOx+ H3EDTA-
1318      1  .0        .0        .0        .0       AmOx+ H2EDTA=
1319      1  .0        .0        .0        .0       AmOx+ HEDTA=-
1320      1  .0        .0        .0        .0       AmOx+ EDTA=-
1321      1  .0        .0        .0        .0       AmOx+ AmEDTA=-
1322      1  .0        .0        .0        .0       AmOx+ NpO2Cit=
1323      1  .0        .0        .0        .0       AmOx+ NpO2EDTA=-
1324      1  .0        .0        .0        .0       AmOx+ NpO2Ox-
1325      1  .0        .0        .0        .0       AmOx+ U(OH)4(CO3)2=-
1326      1  .0        .0        .0        .0       AmOx+ U(CO3)5=-=
1327      1  .0        .0        .0        .0       AmOx+ U(SO4)3=
1328      1  .0        .0        .0        .0       AmOx+ Pu(CO3)2-
1329      1  .0        .0        .0        .0       AmOx+ Pu(CO3)3=-
1330      1  .0        .0        .0        .0       AmOx+ PuEDTA-
1331      1  .0        .0        .0        .0       AmOx+ CaCit-
1332      1  .0        .0        .0        .0       AmOx+ CaEDTA=
1333      1  .0        .0        .0        .0       AmOx+ UnuAn#2-
1334      1  .0        .0        .0        .0       AmOx+ UnuAn#3-
1335      1  .0        .0        .0        .0       AmOx+ UnuAn#4-
1336      1  .0        .0        .0        .0       AmOx+ U(OH)2(CO3)2=
1337      1  .0        .0        .0        .0       AmOx+ MgCit-
1338      1  .0        .0        .0        .0       AmOx+ MgEDTA=
1339      1  .0        .0        .0        .0       AmOx+ UnuAn#1-
1340
1341      1 -.604     -1.607     .0        .0       UCit+ Cl-
1342      1  .0        .0        .0        .0       UCit+ SO4=
1343      1  .0        .0        .0        .0       UCit+ HSO4-
1344      1  .0        .0        .0        .0       UCit+ OH-
1345      1  .0        .0        .0        .0       UCit+ HCO3-
1346      1  .0        .0        .0        .0       UCit+ CO3=
1347      1  .0        .0        .0        .0       UCit+ B(OH)4-
1348      1  .0        .0        .0        .0       UCit+ B3O3(OH)4-
1349      1  .0        .0        .0        .0       UCit+ B4O5(OH)4=
1350      1  .0        .0        .0        .0       UCit+ Br-
1351      1  .0        .0        .0        .0       UCit+ Am(CO3)2-
1352      1  .0        .0        .0        .0       UCit+ Am(CO3)3=-
1353      1  .0        .0        .0        .0       UCit+ ClO4-
1354      1  .0        .0        .0        .0       UCit+ NpO2(OH)2-
1355      1  .0        .0        .0        .0       UCit+ NpO2CO3-
1356      1  .0        .0        .0        .0       UCit+ NpO2(CO3)2=-
1357      1  .0        .0        .0        .0       UCit+ NpO2(CO3)3=-=
1358      1  .0        .0        .0        .0       UCit+ H2PO4-
1359      1  .0        .0        .0        .0       UCit+ HPO4=
1360      1  .0        .0        .0        .0       UCit+ PO4=-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
1381     1  .0        .0        .0        .0        UCit+ Th(SO4)3=
1382     1  .0        .0        .0        .0        UCit+ Th(OH)3(CO3)-
1383     1  .0        .0        .0        .0        UCit+ Th(CO3)5===
1384     1  .0        .0        .0        .0        UCit+ HOx-
1385     1  .0        .0        .0        .0        UCit+ Ox=
1386     1  .0        .0        .0        .0        UCit+ Ac-
1387     1  .0        .0        .0        .0        UCit+ Lac-
1388     1  .0        .0        .0        .0        UCit+ H2Cit-
1389     1  .0        .0        .0        .0        UCit+ HCit=
1390     1  .0        .0        .0        .0        UCit+ Cit---
1391     1  .0        .0        .0        .0        UCit+ H3EDTA-
1392     1  .0        .0        .0        .0        UCit+ H2EDTA=
1393     1  .0        .0        .0        .0        UCit+ HEDTA=-
1394     1  .0        .0        .0        .0        UCit+ EDTA==
1395     1  .0        .0        .0        .0        UCit+ AmEDTA=-
1396     1  .0        .0        .0        .0        UCit+ NpO2Cit=
1397     1  .0        .0        .0        .0        UCit+ NpO2EDTA==-
1398     1  .0        .0        .0        .0        UCit+ NpO2Ox-
1399     1  .0        .0        .0        .0        UCit+ U(OH)4(CO3)2==
1400     1  .0        .0        .0        .0        UCit+ U(CO3)5===
1401     1  .0        .0        .0        .0        UCit+ U(SO4)3=
1402     1  .0        .0        .0        .0        UCit+ Pu(CO3)2-
1403     1  .0        .0        .0        .0        UCit+ Pu(CO3)3=-
1404     1  .0        .0        .0        .0        UCit+ PuEDTA-
1405     1  .0        .0        .0        .0        UCit+ CaCit-
1406     1  .0        .0        .0        .0        UCit+ CaEDTA=
1407     1  .0        .0        .0        .0        UCit+ UnuAn#2-
1408     1  .0        .0        .0        .0        UCit+ UnuAn#3-
1409     1  .0        .0        .0        .0        UCit+ UnuAn#4-
1410     1  .0        .0        .0        .0        UCit+ U(OH)2(CO3)2=
1411     1  .0        .0        .0        .0        UCit+ MgCit-
1412     1  .0        .0        .0        .0        UCit+ MgEDTA=
1413     1  .0        .0        .0        .0        UCit+ UnuAn#1-
1414
1415     1  .2138     5.371     .0        .0        ULac+++ Cl-
1416     3  .0        .0        .0        .0        ULac+++ SO4=
1417     1  .0        .0        .0        .0        ULac+++ HSO4-
1418     1  .0        .0        .0        .0        ULac+++ OH-
1419     1  .0        .0        .0        .0        ULac+++ HCO3-
1420     3  .0        .0        .0        .0        ULac+++ CO3=
1421     1  .0        .0        .0        .0        ULac+++ B(OH)4-
1422     1  .0        .0        .0        .0        ULac+++ B3O3(OH)4-
1423     3  .0        .0        .0        .0        ULac+++ B4O5(OH)4=
1424     1  .0        .0        .0        .0        ULac+++ Br-
1425     1  .0        .0        .0        .0        ULac+++ Am(CO3)2-
1426     3  .0        .0        .0        .0        ULac+++ Am(CO3)3=-
1427     1  .0        .0        .0        .0        ULac+++ ClO4-
1428     1  .0        .0        .0        .0        ULac+++ NpO2(OH)2-
1429     1  .0        .0        .0        .0        ULac+++ NpO2CO3-
1430     1  .0        .0        .0        .0        ULac+++ NpO2(CO3)2=-
1431     3  .0        .0        .0        .0        ULac+++ NpO2(CO3)3==-
1432     1  .0        .0        .0        .0        ULac+++ H2PO4-
1433     3  .0        .0        .0        .0        ULac+++ HPO4=
1434     3  .0        .0        .0        .0        ULac+++ PO4---
1435     3  .0        .0        .0        .0        ULac+++ Th(SO4)3=
1436     1  .0        .0        .0        .0        ULac+++ Th(OH)3(CO3)-
1437     3  .0        .0        .0        .0        ULac+++ Th(CO3)5===
1438     1  .0        .0        .0        .0        ULac+++ HOx-
1439     3  .0        .0        .0        .0        ULac+++ Ox=
1440     1  .0        .0        .0        .0        ULac+++ Ac-
1441     1  .0        .0        .0        .0        ULac+++ Lac-
1442     1  .0        .0        .0        .0        ULac+++ H2Cit-
1443     3  .0        .0        .0        .0        ULac+++ HCit=
1444     3  .0        .0        .0        .0        ULac+++ Cit---
1445     3  .0        .0        .0        .0        ULac+++ H3EDTA-
1446     3  .0        .0        .0        .0        ULac+++ H2EDTA=
1447     3  .0        .0        .0        .0        ULac+++ HEDTA=-
1448     3  .0        .0        .0        .0        ULac+++ EDTA==
1449     3  .0        .0        .0        .0        ULac+++ AmEDTA=-
1450     3  .0        .0        .0        .0        ULac+++ NpO2Cit=
1451     3  .0        .0        .0        .0        ULac+++ NpO2EDTA==-
1452     1  .0        .0        .0        .0        ULac+++ NpO2Ox-
1453     3  .0        .0        .0        .0        ULac+++ U(OH)4(CO3)2==
1454     3  .0        .0        .0        .0        ULac+++ U(CO3)5===
1455     3  .0        .0        .0        .0        ULac+++ U(SO4)3=
1456     1  .0        .0        .0        .0        ULac+++ Pu(CO3)2-
1457     3  .0        .0        .0        .0        ULac+++ Pu(CO3)3=-
1458     1  .0        .0        .0        .0        ULac+++ PuEDTA-
1459     1  .0        .0        .0        .0        ULac+++ CaCit-
1460     3  .0        .0        .0        .0        ULac+++ CaEDTA=
1461     1  .0        .0        .0        .0        ULac+++ UnuAn#2-
1462     1  .0        .0        .0        .0        ULac+++ UnuAn#3-
1463     1  .0        .0        .0        .0        ULac+++ UnuAn#4-
1464     3  .0        .0        .0        .0        ULac+++ U(OH)2(CO3)2=
1465     3  .0        .0        .0        .0        ULac+++ MgCit-
1466     1  .0        .0        .0        .0        ULac+++ MgEDTA=
1467     2  .0        .0        .0        .0        ULac+++ UnuAn#1-
1468     3  .0        .0        .0        .0
1469     2  .0        .0        .0        .0        UOx++ Cl-
1470     1  .0        .0        .0        .0        UOx++ SO4=
1471     3  .0        .0        .0        .0        UOx++ HSO4-
1472     1  .0        .0        .0        .0        UOx++ OH-
1473     2  .0        .0        .0        .0        UOx++ HCO3-
1474     1  .0        .0        .0        .0        UOx++ CO3=
1475     1  .0        .0        .0        .0        UOx++ B(OH)4-
1476     1  .0        .0        .0        .0        UOx++ B3O3(OH)4-
1477     2  .0        .0        .0        .0        UOx++ B4O5(OH)4=
1478     3  .0        .0        .0        .0        UOx++ Br-
1479     3  .0        .0        .0        .0        UOx++ Am(CO3)2-
1480     3  .0        .0        .0        .0        UOx++ Am(CO3)3=-
1481     3  .0        .0        .0        .0        UOx++ ClO4-
1482     3  .0        .0        .0        .0        UOx++ NpO2(OH)2-
1483     3  .0        .0        .0        .0        UOx++ NpO2CO3-
1484     3  .0        .0        .0        .0        UOx++ NpO2(CO3)2=-
1485     3  .0        .0        .0        .0        UOx++ NpO2(CO3)3==-
1486     1  .0        .0        .0        .0        UOx++ H2PO4-
1487     2  .0        .0        .0        .0        UOx++ HPO4=
1488     3  .0        .0        .0        .0        UOx++ PO4---
1489     2  .0        .0        .0        .0        UOx++ Th(SO4)3=
1490     1  .0        .0        .0        .0        UOx++ Th(OH)3(CO3)-
1491     3  .0        .0        .0        .0        UOx++ Th(CO3)5===
1492     1  .0        .0        .0        .0        UOx++ HOx-
1493     2  .0        .0        .0        .0        UOx++ Ox=
1494     1  .0        .0        .0        .0        UOx++ Ac-
1495     1  .0        .0        .0        .0        UOx++ Lac-
1496     1  .0        .0        .0        .0        UOx++ H2Cit-
1497     2  .0        .0        .0        .0        UOx++ HCit=
1498     3  .0        .0        .0        .0        UOx++ Cit---
1499     3  .0        .0        .0        .0        UOx++ H3EDTA-
1500     3  .0        .0        .0        .0        UOx++ H2EDTA=
1501     3  .0        .0        .0        .0        UOx++ HEDTA=-
1502     3  .0        .0        .0        .0        UOx++ EDTA==
1503     3  .0        .0        .0        .0        UOx++ AmEDTA=-
1504     3  .0        .0        .0        .0        UOx++ NpO2Cit=
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
1485      3  .0       .0       .0       .0       UOx++ NpO2EDTA=-
1486      1  .0       .0       .0       .0       UOx++ NpO2Ox-
1487      3  .0       .0       .0       .0       UOx++ U(OH)4(CO3)2=
1488      3  .0       .0       .0       .0       UOx++ U(CO3)5---
1489      2  .0       .0       .0       .0       UOx++ U(SO4)3=
1490      1  .0       .0       .0       .0       UOx++ Pu(CO3)2-
1491      2  .0       .0       .0       .0       UOx++ Pu(CO3)3=-
1492      1  .0       .0       .0       .0       UOx++ PuEDTA-
1493      1  .0       .0       .0       .0       UOx++ CaCit-
1494      2  .0       .0       .0       .0       UOx++ CaEDTA=
1495      3  .0       .0       .0       .0       UOx++ UnuAn#2-
1496      3  .0       .0       .0       .0       UOx++ UnuAn#3-
1497      3  .0       .0       .0       .0       UOx++ UnuAn#4-
1498      2  .0       .0       .0       .0       UOx++ U(OH)2(CO3)2=
1499      1  .0       .0       .0       .0       UOx++ MgCit-
1500      2  .0       .0       .0       .0       UOx++ MgEDTA=
1501      1  .0       .0       .0       .0       UOx++ UnuAn#1-
1502
1503      1  1.239    4.934    .0       .0       ThAc+++ Cl-              RCM96
1504      3  .0       .0       .0       .0       ThAc+++ SO4=
1505      1  .0       .0       .0       .0       ThAc+++ HSO4-
1506      1  .0       .0       .0       .0       ThAc+++ OH-
1507      1  .0       .0       .0       .0       ThAc+++ HCO3-
1508      3  .0       .0       .0       .0       ThAc+++ CO3=
1509      1  .0       .0       .0       .0       ThAc+++ B(OH)4-
1510      1  .0       .0       .0       .0       ThAc+++ B3O3(OH)4-
1511      3  .0       .0       .0       .0       ThAc+++ B4O5(OH)4=
1512      1  .0       .0       .0       .0       ThAc+++ Br-
1513      1  .0       .0       .0       .0       ThAc+++ Am(CO3)2-
1514      3  .0       .0       .0       .0       ThAc+++ Am(CO3)3=-
1515      1  .0       .0       .0       .0       ThAc+++ ClO4-
1516      1  .0       .0       .0       .0       ThAc+++ NpO2(OH)2-
1517      1  .0       .0       .0       .0       ThAc+++ NpO2CO3-
1518      3  .0       .0       .0       .0       ThAc+++ NpO2(CO3)2=-
1519      3  .0       .0       .0       .0       ThAc+++ NpO2(CO3)3=--
1520      1  .0       .0       .0       .0       ThAc+++ H2PO4-
1521      3  .0       .0       .0       .0       ThAc+++ HPO4=
1522      3  .0       .0       .0       .0       ThAc+++ PO4=-
1523      3  .0       .0       .0       .0       ThAc+++ Th(SO4)3=
1524      1  .0       .0       .0       .0       ThAc+++ Th(OH)3(CO3)-
1525      3  .0       .0       .0       .0       ThAc+++ Th(CO3)5---
1526      1  .0       .0       .0       .0       ThAc+++ HOx-
1527      3  .0       .0       .0       .0       ThAc+++ Ox=
1528      1  .0       .0       .0       .0       ThAc+++ Ac-
1529      1  .0       .0       .0       .0       ThAc+++ Lac-
1530      1  .0       .0       .0       .0       ThAc+++ H2Cit-
1531      3  .0       .0       .0       .0       ThAc+++ HCit=
1532      3  .0       .0       .0       .0       ThAc+++ Cit---
1533      3  .0       .0       .0       .0       ThAc+++ H3EDTA-
1534      3  .0       .0       .0       .0       ThAc+++ H2EDTA=
1535      3  .0       .0       .0       .0       ThAc+++ HEDTA=-
1536      3  .0       .0       .0       .0       ThAc+++ EDTA==
1537      3  .0       .0       .0       .0       ThAc+++ AmEDTA=-
1538      3  .0       .0       .0       .0       ThAc+++ NpO2Cit=
1539      3  .0       .0       .0       .0       ThAc+++ NpO2EDTA==-
1540      1  .0       .0       .0       .0       ThAc+++ NpO2Ox-
1541      3  .0       .0       .0       .0       ThAc+++ U(OH)4(CO3)2==
1542      3  .0       .0       .0       .0       ThAc+++ U(CO3)5---
1543      3  .0       .0       .0       .0       ThAc+++ U(SO4)3=
1544      1  .0       .0       .0       .0       ThAc+++ Pu(CO3)2-
1545      3  .0       .0       .0       .0       ThAc+++ Pu(CO3)3=-
1546      1  .0       .0       .0       .0       ThAc+++ PuEDTA-
1547      1  .0       .0       .0       .0       ThAc+++ CaCit-
1548      3  .0       .0       .0       .0       ThAc+++ CaEDTA=
1549      3  .0       .0       .0       .0       ThAc+++ UnuAn#2-
1550      3  .0       .0       .0       .0       ThAc+++ UnuAn#3-
1551      3  .0       .0       .0       .0       ThAc+++ UnuAn#4-
1552      3  .0       .0       .0       .0       ThAc+++ U(OH)2(CO3)2=
1553      1  .0       .0       .0       .0       ThAc+++ MgCit-
1554      3  .0       .0       .0       .0       ThAc+++ MgEDTA=
1555      1  .0       .0       .0       .0       ThAc+++ UnuAn#1-
1556
1557      1  -.604    -1.607   .0       .0       ThCit+ Cl-               RCM96
1558      1  .0       .0       .0       .0       ThCit+ SO4=
1559      1  .0       .0       .0       .0       ThCit+ HSO4-
1560      1  .0       .0       .0       .0       ThCit+ OH-
1561      1  .0       .0       .0       .0       ThCit+ HCO3-
1562      1  .0       .0       .0       .0       ThCit+ CO3=
1563      1  .0       .0       .0       .0       ThCit+ B(OH)4-
1564      1  .0       .0       .0       .0       ThCit+ B3O3(OH)4-
1565      1  .0       .0       .0       .0       ThCit+ B4O5(OH)4=
1566      1  .0       .0       .0       .0       ThCit+ Br-
1567      1  .0       .0       .0       .0       ThCit+ Am(CO3)2-
1568      1  .0       .0       .0       .0       ThCit+ Am(CO3)3=-
1569      1  .0       .0       .0       .0       ThCit+ ClO4-
1570      1  .0       .0       .0       .0       ThCit+ NpO2(OH)2-
1571      1  .0       .0       .0       .0       ThCit+ NpO2CO3-
1572      1  .0       .0       .0       .0       ThCit+ NpO2(CO3)2=-
1573      1  .0       .0       .0       .0       ThCit+ NpO2(CO3)3==-
1574      1  .0       .0       .0       .0       ThCit+ H2PO4-
1575      1  .0       .0       .0       .0       ThCit+ HPO4=
1576      1  .0       .0       .0       .0       ThCit+ PO4=-
1577      1  .0       .0       .0       .0       ThCit+ Th(SO4)3=
1578      1  .0       .0       .0       .0       ThCit+ Th(OH)3(CO3)-
1579      1  .0       .0       .0       .0       ThCit+ Th(CO3)5---
1580      1  .0       .0       .0       .0       ThCit+ HOx-
1581      1  .0       .0       .0       .0       ThCit+ Ox=
1582      1  .0       .0       .0       .0       ThCit+ Ac-
1583      1  .0       .0       .0       .0       ThCit+ Lac-
1584      1  .0       .0       .0       .0       ThCit+ H2Cit-
1585      1  .0       .0       .0       .0       ThCit+ HCit=
1586      1  .0       .0       .0       .0       ThCit+ Cit---
1587      1  .0       .0       .0       .0       ThCit+ H3EDTA-
1588      1  .0       .0       .0       .0       ThCit+ H2EDTA=
1589      1  .0       .0       .0       .0       ThCit+ HEDTA=-
1590      1  .0       .0       .0       .0       ThCit+ EDTA==
1591      1  .0       .0       .0       .0       ThCit+ AmEDTA=-
1592      1  .0       .0       .0       .0       ThCit+ NpO2Cit=
1593      1  .0       .0       .0       .0       ThCit+ NpO2EDTA==-
1594      1  .0       .0       .0       .0       ThCit+ NpO2Ox-
1595      1  .0       .0       .0       .0       ThCit+ U(OH)4(CO3)2==
1596      1  .0       .0       .0       .0       ThCit+ U(CO3)5---
1597      1  .0       .0       .0       .0       ThCit+ U(SO4)3=
1598      1  .0       .0       .0       .0       ThCit+ Pu(CO3)2-
1599      1  .0       .0       .0       .0       ThCit+ Pu(CO3)3=-
1600      1  .0       .0       .0       .0       ThCit+ PuEDTA-
1601      1  .0       .0       .0       .0       ThCit+ CaCit-
1602      1  .0       .0       .0       .0       ThCit+ CaEDTA=
1603      1  .0       .0       .0       .0       ThCit+ UnuAn#2-
1604      1  .0       .0       .0       .0       ThCit+ UnuAn#3-
1605      1  .0       .0       .0       .0       ThCit+ UnuAn#4-
1606      1  .0       .0       .0       .0       ThCit+ U(OH)2(CO3)2=
1607      1  .0       .0       .0       .0       ThCit+ MgCit-
1608      1  .0       .0       .0       .0       ThCit+ MgEDTA=
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
1609    1  .0        .0        .0        .0      ThCit+ UnuAn#1-
1610
1611    1  .2138     5.371     .0        .0      ThLac+++ Cl-          RCM96
1612    3  .0        .0        .0        .0      ThLac+++ SO4=
1613    1  .0        .0        .0        .0      ThLac+++ HSO4-
1614    1  .0        .0        .0        .0      ThLac+++ OH-
1615    1  .0        .0        .0        .0      ThLac+++ HCO3-
1616    3  .0        .0        .0        .0      ThLac+++ CO3=
1617    1  .0        .0        .0        .0      ThLac+++ B(OH)4-
1618    1  .0        .0        .0        .0      ThLac+++ B3O3(OH)4-
1619    3  .0        .0        .0        .0      ThLac+++ B4O5(OH)4=
1620    1  .0        .0        .0        .0      ThLac+++ Br-
1621    1  .0        .0        .0        .0      ThLac+++ Am(CO3)2-
1622    3  .0        .0        .0        .0      ThLac+++ Am(CO3)3=-
1623    1  .0        .0        .0        .0      ThLac+++ ClO4-
1624    1  .0        .0        .0        .0      ThLac+++ NpO2(OH)2-
1625    1  .0        .0        .0        .0      ThLac+++ NpO2CO3-
1626    3  .0        .0        .0        .0      ThLac+++ NpO2(CO3)2=-
1627    3  .0        .0        .0        .0      ThLac+++ NpO2(CO3)3=--
1628    1  .0        .0        .0        .0      ThLac+++ H2PO4-
1629    3  .0        .0        .0        .0      ThLac+++ HPO4=
1630    3  .0        .0        .0        .0      ThLac+++ PO4=-
1631    3  .0        .0        .0        .0      ThLac+++ Th(SO4)3=
1632    1  .0        .0        .0        .0      ThLac+++ Th(OH)3(CO3)-
1633    3  .0        .0        .0        .0      ThLac+++ Th(CO3)5=--
1634    1  .0        .0        .0        .0      ThLac+++ HOx-
1635    3  .0        .0        .0        .0      ThLac+++ Ox=
1636    1  .0        .0        .0        .0      ThLac+++ Ac-
1637    1  .0        .0        .0        .0      ThLac+++ Lac-
1638    1  .0        .0        .0        .0      ThLac+++ H2Cit-
1639    3  .0        .0        .0        .0      ThLac+++ HCit=
1640    3  .0        .0        .0        .0      ThLac+++ Cit=-
1641    3  .0        .0        .0        .0      ThLac+++ H3EDTA-
1642    3  .0        .0        .0        .0      ThLac+++ H2EDTA=
1643    3  .0        .0        .0        .0      ThLac+++ HEDTA=-
1644    3  .0        .0        .0        .0      ThLac+++ EDTA==
1645    3  .0        .0        .0        .0      ThLac+++ AmEDTA=-
1646    3  .0        .0        .0        .0      ThLac+++ NpO2Cit=
1647    3  .0        .0        .0        .0      ThLac+++ NpO2EDTA==-
1648    1  .0        .0        .0        .0      ThLac+++ NpO2Ox-
1649    3  .0        .0        .0        .0      ThLac+++ U(OH)4(CO3)2==
1650    3  .0        .0        .0        .0      ThLac+++ U(CO3)5===
1651    3  .0        .0        .0        .0      ThLac+++ U(SO4)3=
1652    1  .0        .0        .0        .0      ThLac+++ Pu(CO3)2-
1653    3  .0        .0        .0        .0      ThLac+++ Pu(CO3)3=-
1654    1  .0        .0        .0        .0      ThLac+++ PuEDTA-
1655    1  .0        .0        .0        .0      ThLac+++ CaCit-
1656    3  .0        .0        .0        .0      ThLac+++ CaEDTA=
1657    3  .0        .0        .0        .0      ThLac+++ UnuAn#2-
1658    1  .0        .0        .0        .0      ThLac+++ UnuAn#3-
1659    3  .0        .0        .0        .0      ThLac+++ UnuAn#4-
1660    3  .0        .0        .0        .0      ThLac+++ U(OH)2(CO3)2=
1661    1  .0        .0        .0        .0      ThLac+++ MgCit-
1662    3  .0        .0        .0        .0      ThLac+++ MgEDTA=
1663    1  .0        .0        .0        .0      ThLac+++ UnuAn#1-
1664
1665    1 -0.6       3.0       .0        0.2     AmOH++ Cl-    FKPKH94
1666    2  .0        .0        .0        .0      AmOH++ SO4=
1667    1  .0        .0        .0        .0      AmOH++ HSO4-
1668    1  .0        .0        .0        .0      AmOH++ OH-
1669    1  .0        .0        .0        .0      AmOH++ HCO3-
1670    2  .0        .0        .0        .0      AmOH++ CO3=
1671    1  .0        .0        .0        .0      AmOH++ B(OH)4-
1672    1  .0        .0        .0        .0      AmOH++ B3O3(OH)4-
1673    2  .0        .0        .0        .0      AmOH++ B4O5(OH)4=
1674    1  .0        .0        .0        .0      AmOH++ Br-
1675    1  .0        .0        .0        .0      AmOH++ Am(CO3)2-
1676    3  .0        .0        .0        .0      AmOH++ Am(CO3)3=-
1677    1  .0        .0        .0        .0      AmOH++ ClO4-
1678    1  .0        .0        .0        .0      AmOH++ NpO2(OH)2-
1679    1  .0        .0        .0        .0      AmOH++ NpO2CO3-
1680    3  .0        .0        .0        .0      AmOH++ NpO2(CO3)2=-
1681    3  .0        .0        .0        .0      AmOH++ NpO2(CO3)3=-
1682    1  .0        .0        .0        .0      AmOH++ H2PO4-
1683    2  .0        .0        .0        .0      AmOH++ HPO4=
1684    3  .0        .0        .0        .0      AmOH++ PO4=-
1685    2  .0        .0        .0        .0      AmOH++ Th(SO4)3=
1686    1  .0        .0        .0        .0      AmOH++ Th(OH)3(CO3)-
1687    3  .0        .0        .0        .0      AmOH++ Th(CO3)5===
1688    1  .0        .0        .0        .0      AmOH++ HOx-
1689    2  .0        .0        .0        .0      AmOH++ Ox=
1690    1  .0        .0        .0        .0      AmOH++ Ac-
1691    1  .0        .0        .0        .0      AmOH++ Lac-
1692    1  .0        .0        .0        .0      AmOH++ H2Cit-
1693    2  .0        .0        .0        .0      AmOH++ HCit=
1694    3  .0        .0        .0        .0      AmOH++ Cit=-
1695    3  .0        .0        .0        .0      AmOH++ H3EDTA-
1696    3  .0        .0        .0        .0      AmOH++ H2EDTA=
1697    3  .0        .0        .0        .0      AmOH++ HEDTA=-
1698    3  .0        .0        .0        .0      AmOH++ EDTA==
1699    3  .0        .0        .0        .0      AmOH++ AmEDTA=-
1700    3  .0        .0        .0        .0      AmOH++ NpO2Cit=
1701    3  .0        .0        .0        .0      AmOH++ NpO2EDTA==-
1702    1  .0        .0        .0        .0      AmOH++ NpO2Ox-
1703    3  .0        .0        .0        .0      AmOH++ U(OH)4(CO3)2==
1704    3  .0        .0        .0        .0      AmOH++ U(CO3)5===
1705    2  .0        .0        .0        .0      AmOH++ U(SO4)3=
1706    1  .0        .0        .0        .0      AmOH++ Pu(CO3)2-
1707    2  .0        .0        .0        .0      AmOH++ Pu(CO3)3=-
1708    1  .0        .0        .0        .0      AmOH++ PuEDTA-
1709    1  .0        .0        .0        .0      AmOH++ CaCit-
1710    2  .0        .0        .0        .0      AmOH++ CaEDTA=
1711    1  .0        .0        .0        .0      AmOH++ UnuAn#2-
1712    1  .0        .0        .0        .0      AmOH++ UnuAn#3-
1713    2  .0        .0        .0        .0      AmOH++ UnuAn#4-
1714    2  .0        .0        .0        .0      AmOH++ U(OH)2(CO3)2=
1715    1  .0        .0        .0        .0      AmOH++ MgCit-
1716    2  .0        .0        .0        .0      AmOH++ MgEDTA=
1717    1  .0        .0        .0        .0      AmOH++ UnuAn#1-
1718
1719    1 -0.58      -0.9      .0        .0      Am(OH)2+ Cl-    FKPKH94
1720    1  .0        .0        .0        .0      Am(OH)2+ SO4=
1721    1  .0        .0        .0        .0      Am(OH)2+ HSO4-
1722    1  .0        .0        .0        .0      Am(OH)2+ OH-
1723    1  .0        .0        .0        .0      Am(OH)2+ HCO3-
1724    1  .0        .0        .0        .0      Am(OH)2+ CO3=
1725    1  .0        .0        .0        .0      Am(OH)2+ B(OH)4-
1726    1  .0        .0        .0        .0      Am(OH)2+ B3O3(OH)4-
1727    1  .0        .0        .0        .0      Am(OH)2+ B4O5(OH)4=
1728    1  .0        .0        .0        .0      Am(OH)2+ Br-
1729    1  .0        .0        .0        .0      Am(OH)2+ Am(CO3)2-
1730    1  .0        .0        .0        .0      Am(OH)2+ Am(CO3)3=-
1731    1  .0        .0        .0        .0      Am(OH)2+ ClO4-
1732    1  .0        .0        .0        .0      Am(OH)2+ NpO2(OH)2-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
1733    1  .0      .0      .0      .0      Am(OH)2+ NpO2CO3-
1734    1  .0      .0      .0      .0      Am(OH)2+ NpO2(CO3)2=-
1735    1  .0      .0      .0      .0      Am(OH)2+ NpO2(CO3)3===
1736    1  .0      .0      .0      .0      Am(OH)2+ H2PO4-
1737    1  .0      .0      .0      .0      Am(OH)2+ HPO4=
1738    1  .0      .0      .0      .0      Am(OH)2+ PO4=-
1739    1  .0      .0      .0      .0      Am(OH)2+ Th(SO4)3=
1740    1  .0      .0      .0      .0      Am(OH)2+ Th(OH)3(CO3)-
1741    1  .0      .0      .0      .0      Am(OH)2+ Th(CO3)5===
1742    1  .0      .0      .0      .0      Am(OH)2+ HOx-
1743    1  .0      .0      .0      .0      Am(OH)2+ Ox=
1744    1  .0      .0      .0      .0      Am(OH)2+ Ac-
1745    1  .0      .0      .0      .0      Am(OH)2+ Lac-
1746    1  .0      .0      .0      .0      Am(OH)2+ H2Cit-
1747    1  .0      .0      .0      .0      Am(OH)2+ HCit=
1748    1  .0      .0      .0      .0      Am(OH)2+ Cit=-
1749    1  .0      .0      .0      .0      Am(OH)2+ H3EDTA-
1750    1  .0      .0      .0      .0      Am(OH)2+ H2EDTA=
1751    1  .0      .0      .0      .0      Am(OH)2+ HEDTA=-
1752    1  .0      .0      .0      .0      Am(OH)2+ EDTA==
1753    1  .0      .0      .0      .0      Am(OH)2+ AmEDTA=-
1754    1  .0      .0      .0      .0      Am(OH)2+ NpO2Cit=
1755    1  .0      .0      .0      .0      Am(OH)2+ NpO2EDTA==-
1756    1  .0      .0      .0      .0      Am(OH)2+ NpO2Ox-
1757    1  .0      .0      .0      .0      Am(OH)2+ U(OH)4(CO3)2==
1758    1  .0      .0      .0      .0      Am(OH)2+ U(CO3)5===
1759    1  .0      .0      .0      .0      Am(OH)2+ U(SO4)3=
1760    1  .0      .0      .0      .0      Am(OH)2+ Pu(CO3)2-
1761    1  .0      .0      .0      .0      Am(OH)2+ Pu(CO3)3=-
1762    1  .0      .0      .0      .0      Am(OH)2+ PuEDTA-
1763    1  .0      .0      .0      .0      Am(OH)2+ CaCit-
1764    1  .0      .0      .0      .0      Am(OH)2+ CaEDTA=
1765    1  .0      .0      .0      .0      Am(OH)2+ UnuAn#2-
1766    1  .0      .0      .0      .0      Am(OH)2+ UnuAn#3-
1767    1  .0      .0      .0      .0      Am(OH)2+ UnuAn#4-
1768    1  .0      .0      .0      .0      Am(OH)2+ U(OH)2(CO3)2=
1769    1  .0      .0      .0      .0      Am(OH)2+ MgCit-
1770    1  .0      .0      .0      .0      Am(OH)2+ MgEDTA=
1771    1  .0      .0      .0      .0      Am(OH)2+ UnuAn#1-
1772
1773    1  .0      .0      .0      .0      PuCO3+ Cl-
1774    1  .0      .0      .0      .0      PuCO3+ SO4=
1775    1  .0      .0      .0      .0      PuCO3+ HSO4-
1776    1  .0      .0      .0      .0      PuCO3+ OH-
1777    1  .0      .0      .0      .0      PuCO3+ HCO3-
1778    1  .0      .0      .0      .0      PuCO3+ CO3=
1779    1  .0      .0      .0      .0      PuCO3+ B(OH)4-
1780    1  .0      .0      .0      .0      PuCO3+ B3O3(OH)4-
1781    1  .0      .0      .0      .0      PuCO3+ B4O5(OH)4=
1782    1  .0      .0      .0      .0      PuCO3+ Br-
1783    1  .0      .0      .0      .0      PuCO3+ Am(CO3)2-
1784    1  .0      .0      .0      .0      PuCO3+ Am(CO3)3=-
1785    1  .0      .0      .0      .0      PuCO3+ ClO4-
1786    1  .0      .0      .0      .0      PuCO3+ NpO2(OH)2-
1787    1  .0      .0      .0      .0      PuCO3+ NpO2CO3-
1788    1  .0      .0      .0      .0      PuCO3+ NpO2(CO3)2=-
1789    1  .0      .0      .0      .0      PuCO3+ NpO2(CO3)3==-
1790    1  .0      .0      .0      .0      PuCO3+ H2PO4-
1791    1  .0      .0      .0      .0      PuCO3+ HPO4=
1792    1  .0      .0      .0      .0      PuCO3+ PO4=-
1793    1  .0      .0      .0      .0      PuCO3+ Th(SO4)3=
1794    1  .0      .0      .0      .0      PuCO3+ Th(OH)3(CO3)-
1795    1  .0      .0      .0      .0      PuCO3+ Th(CO3)5===
1796    1  .0      .0      .0      .0      PuCO3+ HOx-
1797    1  .0      .0      .0      .0      PuCO3+ Ox=
1798    1  .0      .0      .0      .0      PuCO3+ Ac-
1799    1  .0      .0      .0      .0      PuCO3+ Lac-
1800    1  .0      .0      .0      .0      PuCO3+ H2Cit-
1801    1  .0      .0      .0      .0      PuCO3+ HCit=
1802    1  .0      .0      .0      .0      PuCO3+ Cit=-
1803    1  .0      .0      .0      .0      PuCO3+ H3EDTA-
1804    1  .0      .0      .0      .0      PuCO3+ H2EDTA=
1805    1  .0      .0      .0      .0      PuCO3+ HEDTA=-
1806    1  .0      .0      .0      .0      PuCO3+ EDTA==
1807    1  .0      .0      .0      .0      PuCO3+ AmEDTA=-
1808    1  .0      .0      .0      .0      PuCO3+ NpO2Cit=
1809    1  .0      .0      .0      .0      PuCO3+ NpO2EDTA==-
1810    1  .0      .0      .0      .0      PuCO3+ NpO2Ox-
1811    1  .0      .0      .0      .0      PuCO3+ U(OH)4(CO3)2==
1812    1  .0      .0      .0      .0      PuCO3+ U(CO3)5===
1813    1  .0      .0      .0      .0      PuCO3+ U(SO4)3=
1814    1  .0      .0      .0      .0      PuCO3+ Pu(CO3)2-
1815    1  .0      .0      .0      .0      PuCO3+ Pu(CO3)3=-
1816    1  .0      .0      .0      .0      PuCO3+ PuEDTA-
1817    1  .0      .0      .0      .0      PuCO3+ CaCit-
1818    1  .0      .0      .0      .0      PuCO3+ CaEDTA=
1819    1  .0      .0      .0      .0      PuCO3+ UnuAn#2-
1820    1  .0      .0      .0      .0      PuCO3+ UnuAn#3-
1821    1  .0      .0      .0      .0      PuCO3+ UnuAn#4-
1822    1  .0      .0      .0      .0      PuCO3+ U(OH)2(CO3)2=
1823    1  .0      .0      .0      .0      PuCO3+ MgCit-
1824    1  .0      .0      .0      .0      PuCO3+ MgEDTA=
1825    1  .0      .0      .0      .0      PuCO3+ UnuAn#1-
1826
1827    1 -0.6     3.0     .0      0.2     PuOH++ Cl-   analogy w/Am(III)
1828    2  .0      .0      .0      .0      PuOH++ SO4=
1829    1  .0      .0      .0      .0      PuOH++ HSO4-
1830    1  .0      .0      .0      .0      PuOH++ OH-
1831    1  .0      .0      .0      .0      PuOH++ HCO3-
1832    2  .0      .0      .0      .0      PuOH++ CO3=
1833    1  .0      .0      .0      .0      PuOH++ B(OH)4-
1834    1  .0      .0      .0      .0      PuOH++ B3O3(OH)4-
1835    2  .0      .0      .0      .0      PuOH++ B4O5(OH)4=
1836    1  .0      .0      .0      .0      PuOH++ Br-
1837    1  .0      .0      .0      .0      PuOH++ Am(CO3)2-
1838    3  .0      .0      .0      .0      PuOH++ Am(CO3)3=-
1839    1  .0      .0      .0      .0      PuOH++ ClO4-
1840    1  .0      .0      .0      .0      PuOH++ NpO2(OH)2-
1841    1  .0      .0      .0      .0      PuOH++ NpO2CO3-
1842    3  .0      .0      .0      .0      PuOH++ NpO2(CO3)2=-
1843    3  .0      .0      .0      .0      PuOH++ NpO2(CO3)3==-
1844    1  .0      .0      .0      .0      PuOH++ H2PO4-
1845    2  .0      .0      .0      .0      PuOH++ HPO4=
1846    3  .0      .0      .0      .0      PuOH++ PO4=-
1847    2  .0      .0      .0      .0      PuOH++ Th(SO4)3=
1848    1  .0      .0      .0      .0      PuOH++ Th(OH)3(CO3)-
1849    3  .0      .0      .0      .0      PuOH++ Th(CO3)5===
1850    1  .0      .0      .0      .0      PuOH++ HOx-
1851    2  .0      .0      .0      .0      PuOH++ Ox=
1852    1  .0      .0      .0      .0      PuOH++ Ac-
1853    1  .0      .0      .0      .0      PuOH++ Lac-
1854    1  .0      .0      .0      .0      PuOH++ H2Cit-
1855    2  .0      .0      .0      .0      PuOH++ HCit=
1856    3  .0      .0      .0      .0      PuOH++ Cit=-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
1857    3  .0       .0      .0      .0      PuOH++ H3EDTA-
1858    2  .0       .0      .0      .0      PuOH++ H2EDTA=
1859    3  .0       .0      .0      .0      PuOH++ HEDTA=-
1860    3  .0       .0      .0      .0      PuOH++ EDTA==
1861    3  .0       .0      .0      .0      PuOH++ AmEDTA=-
1862    2  .0       .0      .0      .0      PuOH++ NpO2Cit=
1863    3  .0       .0      .0      .0      PuOH++ NpO2EDTA==-
1864    1  .0       .0      .0      .0      PuOH++ NpO2Ox-
1865    3  .0       .0      .0      .0      PuOH++ U(OH)4(CO3)2==
1866    3  .0       .0      .0      .0      PuOH++ U(CO3)5===
1867    2  .0       .0      .0      .0      PuOH++ U(SO4)3=
1868    1  .0       .0      .0      .0      PuOH++ Pu(CO3)2-
1869    3  .0       .0      .0      .0      PuOH++ Pu(CO3)3=-
1870    3  .0       .0      .0      .0      PuOH++ PuEDTA-
1871    1  .0       .0      .0      .0      PuOH++ CaCit-
1872    2  .0       .0      .0      .0      PuOH++ CaEDTA=
1873    1  .0       .0      .0      .0      PuOH++ UnuAn#2-
1874    1  .0       .0      .0      .0      PuOH++ UnuAn#3-
1875    1  .0       .0      .0      .0      PuOH++ UnuAn#4-
1876    1  .0       .0      .0      .0      PuOH++ U(OH)2(CO3)2=
1877    1  .0       .0      .0      .0      PuOH++ MgCit-
1878    2  .0       .0      .0      .0      PuOH++ MgEDTA=
1879    1  .0       .0      .0      .0      PuOH++ UnuAn#1-
1880
1881    1 -0.58    -0.9      .0      .0      Pu(OH)2+ Cl-   analogy w/Am(III)
1882    1  .0       .0      .0      .0      Pu(OH)2+ SO4=
1883    1  .0       .0      .0      .0      Pu(OH)2+ HSO4-
1884    1  .0       .0      .0      .0      Pu(OH)2+ OH-
1885    1  .0       .0      .0      .0      Pu(OH)2+ HCO3-
1886    1  .0       .0      .0      .0      Pu(OH)2+ CO3=
1887    1  .0       .0      .0      .0      Pu(OH)2+ B(OH)4-
1888    1  .0       .0      .0      .0      Pu(OH)2+ B3O3(OH)4-
1889    1  .0       .0      .0      .0      Pu(OH)2+ B4O5(OH)4=
1890    1  .0       .0      .0      .0      Pu(OH)2+ Br-
1891    1  .0       .0      .0      .0      Pu(OH)2+ Am(CO3)2-
1892    1  .0       .0      .0      .0      Pu(OH)2+ Am(CO3)3=-
1893    1  .0       .0      .0      .0      Pu(OH)2+ ClO4-
1894    1  .0       .0      .0      .0      Pu(OH)2+ NpO2(OH)2-
1895    1  .0       .0      .0      .0      Pu(OH)2+ NpO2CO3-
1896    1  .0       .0      .0      .0      Pu(OH)2+ NpO2(CO3)2=-
1897    1  .0       .0      .0      .0      Pu(OH)2+ NpO2(CO3)3=--
1898    1  .0       .0      .0      .0      Pu(OH)2+ H2PO4-
1899    1  .0       .0      .0      .0      Pu(OH)2+ HPO4=
1900    1  .0       .0      .0      .0      Pu(OH)2+ PO4=-
1901    1  .0       .0      .0      .0      Pu(OH)2+ Th(SO4)3=
1902    1  .0       .0      .0      .0      Pu(OH)2+ Th(OH)3(CO3)-
1903    1  .0       .0      .0      .0      Pu(OH)2+ Th(CO3)5===
1904    1  .0       .0      .0      .0      Pu(OH)2+ HOx-
1905    1  .0       .0      .0      .0      Pu(OH)2+ Ox=
1906    1  .0       .0      .0      .0      Pu(OH)2+ Ac-
1907    1  .0       .0      .0      .0      Pu(OH)2+ Lac-
1908    1  .0       .0      .0      .0      Pu(OH)2+ H2Cit-
1909    1  .0       .0      .0      .0      Pu(OH)2+ HCit=
1910    1  .0       .0      .0      .0      Pu(OH)2+ Cit=-
1911    1  .0       .0      .0      .0      Pu(OH)2+ H3EDTA-
1912    1  .0       .0      .0      .0      Pu(OH)2+ H2EDTA=
1913    1  .0       .0      .0      .0      Pu(OH)2+ HEDTA=-
1914    1  .0       .0      .0      .0      Pu(OH)2+ EDTA==
1915    1  .0       .0      .0      .0      Pu(OH)2+ AmEDTA=-
1916    1  .0       .0      .0      .0      Pu(OH)2+ NpO2Cit=
1917    1  .0       .0      .0      .0      Pu(OH)2+ NpO2EDTA==-
1918    1  .0       .0      .0      .0      Pu(OH)2+ NpO2Ox-
1919    1  .0       .0      .0      .0      Pu(OH)2+ U(OH)4(CO3)2==
1920    1  .0       .0      .0      .0      Pu(OH)2+ U(CO3)5===
1921    1  .0       .0      .0      .0      Pu(OH)2+ U(SO4)3=
1922    1  .0       .0      .0      .0      Pu(OH)2+ Pu(CO3)2-
1923    1  .0       .0      .0      .0      Pu(OH)2+ Pu(CO3)3=-
1924    1  .0       .0      .0      .0      Pu(OH)2+ PuEDTA-
1925    1  .0       .0      .0      .0      Pu(OH)2+ CaCit-
1926    1  .0       .0      .0      .0      Pu(OH)2+ CaEDTA=
1927    1  .0       .0      .0      .0      Pu(OH)2+ UnuAn#2-
1928    1  .0       .0      .0      .0      Pu(OH)2+ UnuAn#3-
1929    1  .0       .0      .0      .0      Pu(OH)2+ UnuAn#4-
1930    1  .0       .0      .0      .0      Pu(OH)2+ U(OH)2(CO3)2=
1931    1  .0       .0      .0      .0      Pu(OH)2+ MgCit-
1932    1  .0       .0      .0      .0      Pu(OH)2+ MgEDTA=
1933    1  .0       .0      .0      .0      Pu(OH)2+ UnuAn#1-
1934
1935    1  .227    2.154    .0     -.102    PuAc++ Cl-          RCM96
1936    2  .0       .0      .0      .0      PuAc++ SO4=
1937    1  .0       .0      .0      .0      PuAc++ HSO4-
1938    1  .0       .0      .0      .0      PuAc++ OH-
1939    1  .0       .0      .0      .0      PuAc++ HCO3-
1940    2  .0       .0      .0      .0      PuAc++ CO3=
1941    1  .0       .0      .0      .0      PuAc++ B(OH)4-
1942    1  .0       .0      .0      .0      PuAc++ B3O3(OH)4-
1943    2  .0       .0      .0      .0      PuAc++ B4O5(OH)4=
1944    1  .0       .0      .0      .0      PuAc++ Br-
1945    1  .0       .0      .0      .0      PuAc++ Am(CO3)2-
1946    3  .0       .0      .0      .0      PuAc++ Am(CO3)3=-
1947    1  .0       .0      .0      .0      PuAc++ ClO4-
1948    1  .0       .0      .0      .0      PuAc++ NpO2(OH)2-
1949    1  .0       .0      .0      .0      PuAc++ NpO2CO3-
1950    3  .0       .0      .0      .0      PuAc++ NpO2(CO3)2=-
1951    3  .0       .0      .0      .0      PuAc++ NpO2(CO3)3=--
1952    1  .0       .0      .0      .0      PuAc++ H2PO4-
1953    2  .0       .0      .0      .0      PuAc++ HPO4=
1954    3  .0       .0      .0      .0      PuAc++ PO4=-
1955    2  .0       .0      .0      .0      PuAc++ Th(SO4)3=
1956    1  .0       .0      .0      .0      PuAc++ Th(OH)3(CO3)-
1957    3  .0       .0      .0      .0      PuAc++ Th(CO3)5===
1958    1  .0       .0      .0      .0      PuAc++ HOx-
1959    2  .0       .0      .0      .0      PuAc++ Ox=
1960    1  .0       .0      .0      .0      PuAc++ Ac-
1961    1  .0       .0      .0      .0      PuAc++ Lac-
1962    1  .0       .0      .0      .0      PuAc++ H2Cit-
1963    2  .0       .0      .0      .0      PuAc++ HCit=
1964    3  .0       .0      .0      .0      PuAc++ Cit=-
1965    3  .0       .0      .0      .0      PuAc++ H3EDTA-
1966    3  .0       .0      .0      .0      PuAc++ H2EDTA=
1967    3  .0       .0      .0      .0      PuAc++ HEDTA=-
1968    3  .0       .0      .0      .0      PuAc++ EDTA==
1969    3  .0       .0      .0      .0      PuAc++ AmEDTA=-
1970    3  .0       .0      .0      .0      PuAc++ NpO2Cit=
1971    3  .0       .0      .0      .0      PuAc++ NpO2EDTA==-
1972    1  .0       .0      .0      .0      PuAc++ NpO2Ox-
1973    3  .0       .0      .0      .0      PuAc++ U(OH)4(CO3)2==
1974    3  .0       .0      .0      .0      PuAc++ U(CO3)5===
1975    2  .0       .0      .0      .0      PuAc++ U(SO4)3=
1976    1  .0       .0      .0      .0      PuAc++ Pu(CO3)2-
1977    2  .0       .0      .0      .0      PuAc++ Pu(CO3)3=-
1978    1  .0       .0      .0      .0      PuAc++ PuEDTA-
1979    1  .0       .0      .0      .0      PuAc++ CaCit-
1980    3  .0       .0      .0      .0      PuAc++ CaEDTA=
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
1981    1  .0        .0        .0        .0      PuAc++ UmuAn#2-
1982    1  .0        .0        .0        .0      PuAc++ UmuAn#3-
1983    2  .0        .0        .0        .0      PuAc++ UmuAn#4-
1984    2  .0        .0        .0        .0      PuAc++ U(OH)2(CO3)2=
1985    1  .0        .0        .0        .0      PuAc++ MgCit-
1986    2  .0        .0        .0        .0      PuAc++ MgEDTA=
1987    1  .0        .0        .0        .0      PuAc++ UmuAn#1-
1988
1989    1 -.3219     .0        .0        .0      PuOx+ Cl-              RCH96
1990    1  .0        .0        .0        .0      PuOx+ SO4=
1991    1  .0        .0        .0        .0      PuOx+ HSO4-
1992    1  .0        .0        .0        .0      PuOx+ OH-
1993    1  .0        .0        .0        .0      PuOx+ HCO3-
1994    1  .0        .0        .0        .0      PuOx+ CO3=
1995    1  .0        .0        .0        .0      PuOx+ B(OH)4-
1996    1  .0        .0        .0        .0      PuOx+ B3O3(OH)4-
1997    1  .0        .0        .0        .0      PuOx+ B4O5(OH)4=
1998    1  .0        .0        .0        .0      PuOx+ Br-
1999    1  .0        .0        .0        .0      PuOx+ Am(CO3)2-
2000    1  .0        .0        .0        .0      PuOx+ Am(CO3)3=-
2001    1  .0        .0        .0        .0      PuOx+ ClO4-
2002    1  .0        .0        .0        .0      PuOx+ NpO2(OH)2-
2003    1  .0        .0        .0        .0      PuOx+ NpO2CO3-
2004    1  .0        .0        .0        .0      PuOx+ NpO2(CO3)2=-
2005    1  .0        .0        .0        .0      PuOx+ NpO2(CO3)3=--
2006    1  .0        .0        .0        .0      PuOx+ H2PO4-
2007    1  .0        .0        .0        .0      PuOx+ HPO4=
2008    1  .0        .0        .0        .0      PuOx+ PO4=-
2009    1  .0        .0        .0        .0      PuOx+ Th(SO4)3=
2010    1  .0        .0        .0        .0      PuOx+ Th(OH)3(CO3)-
2011    1  .0        .0        .0        .0      PuOx+ Th(CO3)5===
2012    1  .0        .0        .0        .0      PuOx+ HOx-
2013    1  .0        .0        .0        .0      PuOx+ Ox=
2014    1  .0        .0        .0        .0      PuOx+ Ac-
2015    1  .0        .0        .0        .0      PuOx+ Lac-
2016    1  .0        .0        .0        .0      PuOx+ H2Cit-
2017    1  .0        .0        .0        .0      PuOx+ HCit=
2018    1  .0        .0        .0        .0      PuOx+ Cit=-
2019    1  .0        .0        .0        .0      PuOx+ H3EDTA-
2020    1  .0        .0        .0        .0      PuOx+ H2EDTA=
2021    1  .0        .0        .0        .0      PuOx+ HEDTA=-
2022    1  .0        .0        .0        .0      PuOx+ EDTA==
2023    1  .0        .0        .0        .0      PuOx+ AmEDTA=-
2024    1  .0        .0        .0        .0      PuOx+ NpO2Cit=
2025    1  .0        .0        .0        .0      PuOx+ NpO2EDTA==-
2026    1  .0        .0        .0        .0      PuOx+ NpO2Ox-
2027    1  .0        .0        .0        .0      PuOx+ U(OH)4(CO3)2==
2028    1  .0        .0        .0        .0      PuOx+ U(CO3)5===
2029    1  .0        .0        .0        .0      PuOx+ U(SO4)3=
2030    1  .0        .0        .0        .0      PuOx+ Pu(CO3)2-
2031    1  .0        .0        .0        .0      PuOx+ Pu(CO3)3=-
2032    1  .0        .0        .0        .0      PuOx+ PuEDTA-
2033    1  .0        .0        .0        .0      PuOx+ CaCit-
2034    1  .0        .0        .0        .0      PuOx+ CaEDTA=
2035    1  .0        .0        .0        .0      PuOx+ UmuAn#2-
2036    1  .0        .0        .0        .0      PuOx+ UmuAn#3-
2037    1  .0        .0        .0        .0      PuOx+ UmuAn#4-
2038    1  .0        .0        .0        .0      PuOx+ U(OH)2(CO3)2=
2039    1  .0        .0        .0        .0      PuOx+ MgCit-
2040    1  .0        .0        .0        .0      PuOx+ MgEDTA=
2041    1  .0        .0        .0        .0      PuOx+ UmuAn#1-
2042
2043    1 -.0572    6.331      .0        .0      PuLac++ Cl-            RCH96
2044    1  .0        .0        .0        .0      PuLac++ SO4=
2045    1  .0        .0        .0        .0      PuLac++ HSO4-
2046    1  .0        .0        .0        .0      PuLac++ OH-
2047    1  .0        .0        .0        .0      PuLac++ HCO3-
2048    1  .0        .0        .0        .0      PuLac++ CO3=
2049    1  .0        .0        .0        .0      PuLac++ B(OH)6-
2050    1  .0        .0        .0        .0      PuLac++ B3O3(OH)4-
2051    1  .0        .0        .0        .0      PuLac++ B4O5(OH)4=
2052    1  .0        .0        .0        .0      PuLac++ Br-
2053    1  .0        .0        .0        .0      PuLac++ Am(CO3)2-
2054    1  .0        .0        .0        .0      PuLac++ Am(CO3)3=-
2055    1  .0        .0        .0        .0      PuLac++ ClO4-
2056    1  .0        .0        .0        .0      PuLac++ NpO2(OH)2-
2057    1  .0        .0        .0        .0      PuLac++ NpO2CO3-
2058    1  .0        .0        .0        .0      PuLac++ NpO2(CO3)2=-
2059    1  .0        .0        .0        .0      PuLac++ NpO2(CO3)3=-
2060    1  .0        .0        .0        .0      PuLac++ H2PO4-
2061    1  .0        .0        .0        .0      PuLac++ HPO4=
2062    1  .0        .0        .0        .0      PuLac++ PO4=-
2063    1  .0        .0        .0        .0      PuLac++ Th(SO4)3=
2064    1  .0        .0        .0        .0      PuLac++ Th(OH)3(CO3)-
2065    1  .0        .0        .0        .0      PuLac++ Th(CO3)5===
2066    1  .0        .0        .0        .0      PuLac++ HOx-
2067    1  .0        .0        .0        .0      PuLac++ Ox=
2068    1  .0        .0        .0        .0      PuLac++ Ac-
2069    1  .0        .0        .0        .0      PuLac++ Lac-
2070    1  .0        .0        .0        .0      PuLac++ H2Cit-
2071    1  .0        .0        .0        .0      PuLac++ HCit=
2072    1  .0        .0        .0        .0      PuLac++ Cit=-
2073    1  .0        .0        .0        .0      PuLac++ H3EDTA-
2074    1  .0        .0        .0        .0      PuLac++ H2EDTA=
2075    1  .0        .0        .0        .0      PuLac++ HEDTA=-
2076    1  .0        .0        .0        .0      PuLac++ EDTA==
2077    1  .0        .0        .0        .0      PuLac++ AmEDTA=-
2078    1  .0        .0        .0        .0      PuLac++ NpO2Cit=
2079    1  .0        .0        .0        .0      PuLac++ NpO2EDTA==-
2080    1  .0        .0        .0        .0      PuLac++ NpO2Ox-
2081    1  .0        .0        .0        .0      PuLac++ U(OH)4(CO3)2=
2082    1  .0        .0        .0        .0      PuLac++ U(CO3)5===
2083    1  .0        .0        .0        .0      PuLac++ U(SO4)3=
2084    1  .0        .0        .0        .0      PuLac++ Pu(CO3)2-
2085    1  .0        .0        .0        .0      PuLac++ Pu(CO3)3=-
2086    1  .0        .0        .0        .0      PuLac++ PuEDTA-
2087    1  .0        .0        .0        .0      PuLac++ CaCit-
2088    1  .0        .0        .0        .0      PuLac++ CaEDTA=
2089    1  .0        .0        .0        .0      PuLac++ UmuAn#2-
2090    1  .0        .0        .0        .0      PuLac++ UmuAn#3-
2091    1  .0        .0        .0        .0      PuLac++ UmuAn#4-
2092    1  .0        .0        .0        .0      PuLac++ U(OH)2(CO3)2=
2093    1  .0        .0        .0        .0      PuLac++ MgCit-
2094    1  .0        .0        .0        .0      PuLac++ MgEDTA=
2095    1  .0        .0        .0        .0      PuLac++ UmuAn#1-
2096
2097    1  .1696     .0        .0        .0      CaAc+ Cl-      analogy w/Mg++
2098    1  .0        .0        .0        .0      CaAc+ SO4=
2099    1  .0        .0        .0        .0      CaAc+ HSO4-
2100    1  .0        .0        .0        .0      CaAc+ OH-
2101    1  .0        .0        .0        .0      CaAc+ HCO3-
2102    1  .0        .0        .0        .0      CaAc+ CO3=
2103    1  .0        .0        .0        .0      CaAc+ B(OH)4-
2104    1  .0        .0        .0        .0      CaAc+ B3O3(OH)4-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
2105      1  .0        .0        .0        .0        CaAc+ B405(OH)4=
2106      1  .0        .0        .0        .0        CaAc+ Br-
2107      1  .0        .0        .0        .0        CaAc+ Am(CO3)2-
2108      1  .0        .0        .0        .0        CaAc+ Am(CO3)3=-
2109      1  .0        .0        .0        .0        CaAc+ Cl04-
2110      1  .0        .0        .0        .0        CaAc+ NpO2(OH)2-
2111      1  .0        .0        .0        .0        CaAc+ NpO2CO3-
2112      1  .0        .0        .0        .0        CaAc+ NpO2(CO3)2=-
2113      1  .0        .0        .0        .0        CaAc+ NpO2(CO3)3=-
2114      1  .0        .0        .0        .0        CaAc+ H2PO4-
2115      1  .0        .0        .0        .0        CaAc+ HPO4=
2116      1  .0        .0        .0        .0        CaAc+ PO4=-
2117      1  .0        .0        .0        .0        CaAc+ Th(SO4)3=
2118      1  .0        .0        .0        .0        CaAc+ Th(OH)3(CO3)-
2119      1  .0        .0        .0        .0        CaAc+ Th(CO3)5=-
2120      1  .0        .0        .0        .0        CaAc+ HOx-
2121      1  .0        .0        .0        .0        CaAc+ Ox=
2122      1  .0        .0        .0        .0        CaAc+ Ac-
2123      1  .0        .0        .0        .0        CaAc+ Lac-
2124      1  .0        .0        .0        .0        CaAc+ H2Cit-
2125      1  .0        .0        .0        .0        CaAc+ HCit=
2126      1  .0        .0        .0        .0        CaAc+ Cit=-
2127      1  .0        .0        .0        .0        CaAc+ H3EDTA-
2128      1  .0        .0        .0        .0        CaAc+ H2EDTA=
2129      1  .0        .0        .0        .0        CaAc+ HEDTA=-
2130      1  .0        .0        .0        .0        CaAc+ EDTA=-
2131      1  .0        .0        .0        .0        CaAc+ AmEDTA=-
2132      1  .0        .0        .0        .0        CaAc+ NpO2Cit=
2133      1  .0        .0        .0        .0        CaAc+ NpO2EDTA=-
2134      1  .0        .0        .0        .0        CaAc+ NpO2Ox-
2135      1  .0        .0        .0        .0        CaAc+ U(OH)4(CO3)2=-
2136      1  .0        .0        .0        .0        CaAc+ U(CO3)5=-=
2137      1  .0        .0        .0        .0        CaAc+ U(SO4)3=
2138      1  .0        .0        .0        .0        CaAc+ Pu(CO3)2-
2139      1  .0        .0        .0        .0        CaAc+ Pu(CO3)3=-
2140      1  .0        .0        .0        .0        CaAc+ PuEDTA-
2141      1  .0        .0        .0        .0        CaAc+ CaCit-
2142      1  .0        .0        .0        .0        CaAc+ CaEDTA=
2143      1  .0        .0        .0        .0        CaAc+ UnuAn#2-
2144      1  .0        .0        .0        .0        CaAc+ UnuAn#3-
2145      1  .0        .0        .0        .0        CaAc+ UnuAn#4-
2146      1  .0        .0        .0        .0        CaAc+ U(OH)2(CO3)2=
2147      1  .0        .0        .0        .0        CaAc+ MgCit-
2148      1  .0        .0        .0        .0        CaAc+ MgEDTA=
2149      1  .0        .0        .0        .0        CaAc+ UnuAn#1-
2150
2151      1  .0        .0        .0        .0        CaLac+ Cl-
2152      1  .0        .0        .0        .0        CaLac+ SO4=
2153      1  .0        .0        .0        .0        CaLac+ HSO4-
2154      1  .0        .0        .0        .0        CaLac+ OH-
2155      1  .0        .0        .0        .0        CaLac+ HCO3-
2156      1  .0        .0        .0        .0        CaLac+ CO3=
2157      1  .0        .0        .0        .0        CaLac+ B(OH)4-
2158      1  .0        .0        .0        .0        CaLac+ B3O3(OH)4-
2159      1  .0        .0        .0        .0        CaLac+ B4O5(OH)4=
2160      1  .0        .0        .0        .0        CaLac+ Br-
2161      1  .0        .0        .0        .0        CaLac+ Am(CO3)2-
2162      1  .0        .0        .0        .0        CaLac+ Am(CO3)3=-
2163      1  .0        .0        .0        .0        CaLac+ Cl04-
2164      1  .0        .0        .0        .0        CaLac+ NpO2(OH)2-
2165      1  .0        .0        .0        .0        CaLac+ NpO2CO3-
2166      1  .0        .0        .0        .0        CaLac+ NpO2(CO3)2=-
2167      1  .0        .0        .0        .0        CaLac+ NpO2(CO3)3=-
2168      1  .0        .0        .0        .0        CaLac+ H2PO4-
2169      1  .0        .0        .0        .0        CaLac+ HPO4=
2170      1  .0        .0        .0        .0        CaLac+ PO4=-
2171      1  .0        .0        .0        .0        CaLac+ Th(SO4)3=
2172      1  .0        .0        .0        .0        CaLac+ Th(OH)3(CO3)-
2173      1  .0        .0        .0        .0        CaLac+ Th(CO3)5=-
2174      1  .0        .0        .0        .0        CaLac+ HOx-
2175      1  .0        .0        .0        .0        CaLac+ Ox=
2176      1  .0        .0        .0        .0        CaLac+ Ac-
2177      1  .0        .0        .0        .0        CaLac+ Lac-
2178      1  .0        .0        .0        .0        CaLac+ H2Cit-
2179      1  .0        .0        .0        .0        CaLac+ HCit=
2180      1  .0        .0        .0        .0        CaLac+ Cit=-
2181      1  .0        .0        .0        .0        CaLac+ H3EDTA-
2182      1  .0        .0        .0        .0        CaLac+ H2EDTA=
2183      1  .0        .0        .0        .0        CaLac+ HEDTA=-
2184      1  .0        .0        .0        .0        CaLac+ EDTA=-
2185      1  .0        .0        .0        .0        CaLac+ AmEDTA=-
2186      1  .0        .0        .0        .0        CaLac+ NpO2Cit=
2187      1  .0        .0        .0        .0        CaLac+ NpO2EDTA=-
2188      1  .0        .0        .0        .0        CaLac+ NpO2Ox-
2189      1  .0        .0        .0        .0        CaLac+ U(OH)4(CO3)2=-
2190      1  .0        .0        .0        .0        CaLac+ U(CO3)5=-=
2191      1  .0        .0        .0        .0        CaLac+ U(SO4)3=
2192      1  .0        .0        .0        .0        CaLac+ Pu(CO3)2-
2193      1  .0        .0        .0        .0        CaLac+ Pu(CO3)3=-
2194      1  .0        .0        .0        .0        CaLac+ PuEDTA-
2195      1  .0        .0        .0        .0        CaLac+ CaCit-
2196      1  .0        .0        .0        .0        CaLac+ CaEDTA=
2197      1  .0        .0        .0        .0        CaLac+ UnuAn#2-
2198      1  .0        .0        .0        .0        CaLac+ UnuAn#3-
2199      1  .0        .0        .0        .0        CaLac+ UnuAn#4-
2200      1  .0        .0        .0        .0        CaLac+ U(OH)2(CO3)2=
2201      1  .0        .0        .0        .0        CaLac+ MgCit-
2202      1  .0        .0        .0        .0        CaLac+ MgEDTA=
2203      1  .0        .0        .0        .0        CaLac+ UnuAn#1-
2204
2205      1  .1696     .0        .0        .0        MgAc+ Cl-          RCH96c
2206      1  .0        .0        .0        .0        MgAc+ SO4=
2207      1  .0        .0        .0        .0        MgAc+ HSO4-
2208      1  .0        .0        .0        .0        MgAc+ OH-
2209      1  .0        .0        .0        .0        MgAc+ HCO3-
2210      1  .0        .0        .0        .0        MgAc+ CO3=
2211      1  .0        .0        .0        .0        MgAc+ B(OH)4-
2212      1  .0        .0        .0        .0        MgAc+ B3O3(OH)4-
2213      1  .0        .0        .0        .0        MgAc+ B4O5(OH)4=
2214      1  .0        .0        .0        .0        MgAc+ Br-
2215      1  .0        .0        .0        .0        MgAc+ Am(CO3)2-
2216      1  .0        .0        .0        .0        MgAc+ Am(CO3)3=-
2217      1  .0        .0        .0        .0        MgAc+ Cl04-
2218      1  .0        .0        .0        .0        MgAc+ NpO2(OH)2-
2219      1  .0        .0        .0        .0        MgAc+ NpO2CO3-
2220      1  .0        .0        .0        .0        MgAc+ NpO2(CO3)2=-
2221      1  .0        .0        .0        .0        MgAc+ NpO2(CO3)3=-
2222      1  .0        .0        .0        .0        MgAc+ H2PO4-
2223      1  .0        .0        .0        .0        MgAc+ HPO4=
2224      1  .0        .0        .0        .0        MgAc+ PO4=-
2225      1  .0        .0        .0        .0        MgAc+ Th(SO4)3=
2226      1  .0        .0        .0        .0        MgAc+ Th(OH)3(CO3)-
2227      1  .0        .0        .0        .0        MgAc+ Th(CO3)5=-
2228      1  .0        .0        .0        .0        MgAc+ HOx-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
2229    1  .0      .0      .0      .0      MgAc+ Ox+
2230    1  .0      .0      .0      .0      MgAc+ Ac-
2231    1  .0      .0      .0      .0      MgAc+ Lac-
2232    1  .0      .0      .0      .0      MgAc+ H2Cit-
2233    1  .0      .0      .0      .0      MgAc+ HCit=
2234    1  .0      .0      .0      .0      MgAc+ Cit=-
2235    1  .0      .0      .0      .0      MgAc+ H3EDTA-
2236    1  .0      .0      .0      .0      MgAc+ H2EDTA=
2237    1  .0      .0      .0      .0      MgAc+ HEDTA=-
2238    1  .0      .0      .0      .0      MgAc+ EDTA==
2239    1  .0      .0      .0      .0      MgAc+ AmEDTA=-
2240    1  .0      .0      .0      .0      MgAc+ NpO2Cit=
2241    1  .0      .0      .0      .0      MgAc+ NpO2EDTA==-
2242    1  .0      .0      .0      .0      MgAc+ NpO2Ox-
2243    1  .0      .0      .0      .0      MgAc+ U(OH)4(CO3)2==
2244    1  .0      .0      .0      .0      MgAc+ U(CO3)5===
2245    1  .0      .0      .0      .0      MgAc+ U(SO4)3=
2246    1  .0      .0      .0      .0      MgAc+ Pu(CO3)2-
2247    1  .0      .0      .0      .0      MgAc+ Pu(CO3)3=-
2248    1  .0      .0      .0      .0      MgAc+ PuEDTA-
2249    1  .0      .0      .0      .0      MgAc+ CaCit-
2250    1  .0      .0      .0      .0      MgAc+ CaEDTA=
2251    1  .0      .0      .0      .0      MgAc+ UnuAn#2-
2252    1  .0      .0      .0      .0      MgAc+ UnuAn#3-
2253    1  .0      .0      .0      .0      MgAc+ UnuAn#4-
2254    1  .0      .0      .0      .0      MgAc+ U(OH)2(CO3)2=
2255    1  .0      .0      .0      .0      MgAc+ MgCit-
2256    1  .0      .0      .0      .0      MgAc+ MgEDTA=
2257    1  .0      .0      .0      .0      MgAc+ UnuAn#1-
2258
2259    1  .0      .0      .0      .0      MgLac+ Cl-
2260    1  .0      .0      .0      .0      MgLac+ SO4=
2261    1  .0      .0      .0      .0      MgLac+ HSO4-
2262    1  .0      .0      .0      .0      MgLac+ OH-
2263    1  .0      .0      .0      .0      MgLac+ HCO3-
2264    1  .0      .0      .0      .0      MgLac+ CO3=
2265    1  .0      .0      .0      .0      MgLac+ B(OH)4-
2266    1  .0      .0      .0      .0      MgLac+ BJO3(OH)4-
2267    1  .0      .0      .0      .0      MgLac+ B4O5(OH)4=
2268    1  .0      .0      .0      .0      MgLac+ Br-
2269    1  .0      .0      .0      .0      MgLac+ Am(CO3)2-
2270    1  .0      .0      .0      .0      MgLac+ Am(CO3)3=-
2271    1  .0      .0      .0      .0      MgLac+ ClO4-
2272    1  .0      .0      .0      .0      MgLac+ NpO2(OH)2-
2273    1  .0      .0      .0      .0      MgLac+ NpO2CO3-
2274    1  .0      .0      .0      .0      MgLac+ NpO2(CO3)2=-
2275    1  .0      .0      .0      .0      MgLac+ NpO2(CO3)3==-
2276    1  .0      .0      .0      .0      MgLac+ H2PO4-
2277    1  .0      .0      .0      .0      MgLac+ HPO4=
2278    1  .0      .0      .0      .0      MgLac+ PO4=-
2279    1  .0      .0      .0      .0      MgLac+ Th(SO4)3=
2280    1  .0      .0      .0      .0      MgLac+ Th(OH)3(CO3)-
2281    1  .0      .0      .0      .0      MgLac+ Th(CO3)5===
2282    1  .0      .0      .0      .0      MgLac+ HOx-
2283    1  .0      .0      .0      .0      MgLac+ Ox=
2284    1  .0      .0      .0      .0      MgLac+ Ac-
2285    1  .0      .0      .0      .0      MgLac+ Lac-
2286    1  .0      .0      .0      .0      MgLac+ H2Cit-
2287    1  .0      .0      .0      .0      MgLac+ HCit=
2288    1  .0      .0      .0      .0      MgLac+ Cit=-
2289    1  .0      .0      .0      .0      MgLac+ H3EDTA-
2290    1  .0      .0      .0      .0      MgLac+ H2EDTA=
2291    1  .0      .0      .0      .0      MgLac+ HEDTA=-
2292    1  .0      .0      .0      .0      MgLac+ EDTA==
2293    1  .0      .0      .0      .0      MgLac+ AmEDTA=-
2294    1  .0      .0      .0      .0      MgLac+ NpO2Cit=
2295    1  .0      .0      .0      .0      MgLac+ NpO2EDTA==-
2296    1  .0      .0      .0      .0      MgLac+ NpO2Ox-
2297    1  .0      .0      .0      .0      MgLac+ U(OH)4(CO3)2==
2298    1  .0      .0      .0      .0      MgLac+ U(CO3)5===
2299    1  .0      .0      .0      .0      MgLac+ U(SO4)3=
2300    1  .0      .0      .0      .0      MgLac+ Pu(CO3)2-
2301    1  .0      .0      .0      .0      MgLac+ Pu(CO3)3=-
2302    1  .0      .0      .0      .0      MgLac+ PuEDTA-
2303    1  .0      .0      .0      .0      MgLac+ CaCit-
2304    1  .0      .0      .0      .0      MgLac+ CaEDTA=
2305    1  .0      .0      .0      .0      MgLac+ UnuAn#2-
2306    1  .0      .0      .0      .0      MgLac+ UnuAn#3-
2307    1  .0      .0      .0      .0      MgLac+ UnuAn#4-
2308    1  .0      .0      .0      .0      MgLac+ U(OH)2(CO3)2=
2309    1  .0      .0      .0      .0      MgLac+ MgCit-
2310    1  .0      .0      .0      .0      MgLac+ MgEDTA=
2311    1  .0      .0      .0      .0      MgLac+ UnuAn#1-
2312
2313    1  .0      .0      .0      .0      UnuCat#1+ Cl-
2314    1  .0      .0      .0      .0      UnuCat#1+ SO4=
2315    1  .0      .0      .0      .0      UnuCat#1+ HSO4-
2316    1  .0      .0      .0      .0      UnuCat#1+ OH-
2317    1  .0      .0      .0      .0      UnuCat#1+ HCO3-
2318    1  .0      .0      .0      .0      UnuCat#1+ CO3=
2319    1  .0      .0      .0      .0      UnuCat#1+ B(OH)4-
2320    1  .0      .0      .0      .0      UnuCat#1+ BJO3(OH)4-
2321    1  .0      .0      .0      .0      UnuCat#1+ B4O5(OH)4=
2322    1  .0      .0      .0      .0      UnuCat#1+ Br-
2323    1  .0      .0      .0      .0      UnuCat#1+ Am(CO3)2-
2324    1  .0      .0      .0      .0      UnuCat#1+ Am(CO3)3=-
2325    1  .0      .0      .0      .0      UnuCat#1+ ClO4-
2326    1  .0      .0      .0      .0      UnuCat#1+ NpO2(OH)2-
2327    1  .0      .0      .0      .0      UnuCat#1+ NpO2CO3-
2328    1  .0      .0      .0      .0      UnuCat#1+ NpO2(CO3)2=-
2329    1  .0      .0      .0      .0      UnuCat#1+ NpO2(CO3)3==-
2330    1  .0      .0      .0      .0      UnuCat#1+ H2PO4-
2331    1  .0      .0      .0      .0      UnuCat#1+ HPO4=
2332    1  .0      .0      .0      .0      UnuCat#1+ PO4=-
2333    1  .0      .0      .0      .0      UnuCat#1+ Th(SO4)3=
2334    1  .0      .0      .0      .0      UnuCat#1+ Th(OH)3(CO3)-
2335    1  .0      .0      .0      .0      UnuCat#1+ Th(CO3)5===
2336    1  .0      .0      .0      .0      UnuCat#1+ HOx-
2337    1  .0      .0      .0      .0      UnuCat#1+ Ox=
2338    1  .0      .0      .0      .0      UnuCat#1+ Ac-
2339    1  .0      .0      .0      .0      UnuCat#1+ Lac-
2340    1  .0      .0      .0      .0      UnuCat#1+ H2Cit-
2341    1  .0      .0      .0      .0      UnuCat#1+ HCit=
2342    1  .0      .0      .0      .0      UnuCat#1+ Cit=-
2343    1  .0      .0      .0      .0      UnuCat#1+ H3EDTA-
2344    1  .0      .0      .0      .0      UnuCat#1+ H2EDTA=
2345    1  .0      .0      .0      .0      UnuCat#1+ HEDTA=-
2346    1  .0      .0      .0      .0      UnuCat#1+ EDTA==
2347    1  .0      .0      .0      .0      UnuCat#1+ AmEDTA=-
2348    1  .0      .0      .0      .0      UnuCat#1+ NpO2Cit=
2349    1  .0      .0      .0      .0      UnuCat#1+ NpO2EDTA==-
2350    1  .0      .0      .0      .0      UnuCat#1+ NpO2Ox-
2351    1  .0      .0      .0      .0      UnuCat#1+ U(OH)4(CO3)2==
2352    1  .0      .0      .0      .0      UnuCat#1+ U(CO3)5===
```

```
1  .0     .0     .0    .0      UnuCat#1+ U(SO4)3=
1  .0     .0     .0    .0      UnuCat#1+ Pu(CO3)2-
1  .0     .0     .0    .0      UnuCat#1+ Pu(CO3)3=-
1  .0     .0     .0    .0      UnuCat#1+ PuEDTA-
1  .0     .0     .0    .0      UnuCat#1+ CaCit-
1  .0     .0     .0    .0      UnuCat#1+ CaEDTA=
1  .0     .0     .0    .0      UnuCat#1+ UnuAn#2-
1  .0     .0     .0    .0      UnuCat#1+ UnuAn#3-
1  .0     .0     .0    .0      UnuCat#1+ UnuAn#4-
1  .0     .0     .0    .0      UnuCat#1+ U(OH)2(CO3)2=
1  .0     .0     .0    .0      UnuCat#1+ MgCit-
1  .0     .0     .0    .0      UnuCat#1+ MgEDTA=
1  .0     .0     .0    .0      UnuCat#1+ UnuAn#1-

-.012 .07  .07 0 .036 0 0 0 0 .42 -.0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na      1 w/2-39) theta  CFN960119,WJ96
      .032   0 0 .005 0 0 0 0   0  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K:      2 w/3-39) theta
          .007 0 .092 0 0 0 0   0  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca:     3 w/4-39) theta
               0 .10  0 0 0 0 .60  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg:     4 w/5-39) theta  CFN960119
                    0 0 0 0 0   0  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH:   5 w/6-39) theta
                      0 0 0 0 .60 .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H :     6 w/7-39) theta  Roy92,WJ96

  0 0 0  0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4:  7 w/8-39) theta
    0 0  0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4:  8 w/9-39) theta
      0  0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++:     9 w/10-39) theta
         0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+:   10 w/11-39) theta
           0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++:   11 w/12-39) theta
               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++:    12 w/13-39) theta
                 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+:    13 w/14-39) theta
                   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++:    14 w/15-39) theta
                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++:   15 w/16-39) theta
                       0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++:   16 w/17-39) theta
                         0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++    17 w/18-39) theta
                           0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++    18 w/19-39) theta
                             0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++   19 w/20-39) theta
                               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+     20 w/21-39) theta
                                 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+     21 w/22-39) theta
                                   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++   22 w/23-39) theta
                                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++     23 w/24-39) theta
                                       0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++   24 w/25-39) theta
                                         0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+    25 w/26-39) theta
                                           0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++  26 w/27-39) theta
                                             0 0 0 0 0 0 0 0 0 0 0 0 AmOH++    27 w/28-39) theta
                                               0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+  28 w/29-39) theta
                                                 0 0 0 0 0 0 0 0 0 0 PuCO3+    29 w/30-39) theta
                                                   0 0 0 0 0 0 0 0 0 PuOH++    30 w/31-39) theta
                                                     0 0 0 0 0 0 0 0 Pu(OH)2+  31 w/32-39) theta
                                                       0 0 0 0 0 0 0 PuAc++    32 w/33-39) theta
                                                         0 0 0 0 0 0 PuOx+     33 w/34-39) theta
                                                           0 0 0 0 0 PuLac++   34 w/35-39) theta
                                                             0 0 0 0 CaAc+     35 w/36-39) theta
                                                               0 0 0 CaLac+    36 w/37-39) theta
                                                                 0 0 MgAc+     37 w/38-39) theta
                                                                   0 MgLac+    38 w/39-39) theta

.02 -.006 -.05 .03 -.02 -.065 .12 .074 0 0 .168  0 -.26 -.21 -.26 -.26 .1 0 0  0 0 5.5 0 0 -.09 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                0 0 0 0 .168 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl
      0 -.013 .01 .02 -.012 .10  .12 0 0 0  .02  0    0    0    0  0 0 0  0 0   0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4
          0   0   0    0    0      0 0 0 0    0  0    0    0    0  0 0 0  0 0   0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 HSO4
              0 .10    0    0      0 0 0 0 -.032  0    0    0    0  0 0 0  0 0   0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 OH
                 -.04  0 -.10 -.087 0 0 0  .095  0    0    0    0  0 0 0  0 0   0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 HCO3

0 0 0 0 0 0 .21 0 0 0 -1.90 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CO3
  0 0 0 0 0   0 0 0 0     0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 B(OH)4
    0 0 0 0   0 0 0 0     0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 B3O3(OH)4
      0 0 0   0 0 0 0     0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 B4O5(OH)4
        0 0   0 0 0 0     0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Br
          0   0 0 0 0     0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(CO3)2-
              0 0 0 0     0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(CO3)3=-
                0 0 0     0 0 0 0 0 0  5.5  .35 0 0 0 .007 .0297 .0921 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4-      FRSMIC96
                  0 0     0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2-
                    0     0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpC-
                          0 0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpC2=-
                            0 0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpC3==-
                              0 0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2PO4-
                                0 0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HPO4=
                                  0 0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PO4=-
                                    0    0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th(SO4)=
                                         0    0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th(OH)3CO3-
                                              0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th(CO3)5===
                                                0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx-
                                                  0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox=
                                                    0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac-
                                                         0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac-
                                                               0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit-
                                                               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HCit=
                                                                 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cit=-
                                                                   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H3EDTA-
                                                                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2EDTA=
                                                                       0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HEDTA=-
                                                                         0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 EDTA==
                                                                           0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmEDTA=-
                                                                             0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2Cit=
                                                                               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2EDTA==-
                                                                                 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2Ox-
                                                                                   0 0 0 0 0 0 0 0 0 0 0 0 0 0 U(OH)3CO3-
                                                                                     0 0 0 0 0 0 0 0 0 0 0 0 0 U(CO3)5===
                                                                                       0 0 0 0 0 0 0 0 0 0 0 0 U(SO4)3=
                                                                                         0 0 0 0 0 0 0 0 0 0 0 Pu(CO3)2-
                                                                                           0 0 0 0 0 0 0 0 0 0 Pu(CO3)3=-
                                                                                             0 0 0 0 0 0 0 0 0 PuEDTA-
                                                                                               0 0 0 0 0 0 0 0 CaCit-
                                                                                                 0 0 0 0 0 0 0 CaEDTA=
                                                                                                   0 0 0 0 0 0 UnuAn#2-
                                                                                                     0 0 0 0 0 UnuAn#3-
                                                                                                       0 0 0 0 UnuAn#4-
                                                                                                         0 0 0 U(OH)2(CO3)2=
                                                                                                           0 0 MgCit-
                                                                                                             0 MgEDTA=

-.0018 -.010    .0 0 -.003 .003 0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-K+:anions psi
 -.007 -.055    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-Ca++:
 -.012 -.015    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-Mg++:
    .0    .0    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-MgOH+:
 -.004    .0 -.0129 0  .0   .0  0 0 0 0 0 0 0 -.016 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-H+:
    .0    .0    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-MgB(OH)4+
    .0    .0    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-CaB(OH)4+
    .0    .0    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-Am+++
    .0    .0    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-AmCO3+
   .21    .0    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-Th++++ CFN960119
    .0    .0    .0 0   .0   .0  0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+-Pu+++
```

```
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--NpO2++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--U++++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--UOH+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--UAc+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--ThOx++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--AmAc++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--AmLac++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--AmOx+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--UCit+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--ULac+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--UOx++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--ThAc+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--ThCit+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--ThLac+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--AmOH++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--Am(OH)2+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--PuCO3+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--PuOH++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--Pu(OH)2+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--PuAc++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--PuOx+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--PuLac++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--CaAc+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--CaLac+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--MgAc+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--MgLac+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Na+--UnuCat#1+

-.025    .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--Ca:
-.022 -.048     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--Mg:
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--MgOH:
-.011  .197 -.0265 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--H :
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--MgB(OH)4+
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--CaB(OH)4+
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--Am+++
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--AmCO3+
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--Th++++
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--Pu+++
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--NpO2++
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--U++++
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--UOH+++
  .0     .0     .0 0   0   0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--UAc+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--ThOx++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--AmAc++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--AmLac++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--AmOx+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--UCit+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--ULac+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--UOx++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--ThAc+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--ThCit+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--ThLac+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--AmOH++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--Am(OH)2+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--PuCO3+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--PuOH++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--Pu(OH)2+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--PuAc++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--PuOx+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--PuLac++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--CaAc+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--CaLac+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--MgAc+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--MgLac+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 K+--UnuCat#1+

-.012  .026     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--Mg:
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--MgOH:
-.015    .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--H :
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--MgB(OH)4+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--Ca++B(OH)4+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--Am+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--AmCO3+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--Th++++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--Pu+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--NpO2++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--U++++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--UOH+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--UAc+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--ThOx++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--AmAc++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--AmLac++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--AmOx+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--UCit+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--ULac+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--UOx++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--ThAc+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--ThCit+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--ThLac+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--AmOH++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--Am(OH)2+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--PuCO3+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--PuOH++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--Pu(OH)2+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--PuAc++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--PuOx+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--PuLac++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--CaAc+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca++--CaLac+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca+-MgAc+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca+-MgLac+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ca+-UnuCat#1+

 .028    .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--MgOH:
-.011    .0 -.0178 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--H :
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--MgB(OH)4+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--CaB(OH)4+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--Am+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--AmCO3+
  .21    .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--Th++++ CFN960119
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--Pu+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--NpO2++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--U++++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--UOH+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--UAc+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--ThOx++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--AmAc++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--AmLac++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--AmOx+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--UCit+
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--ULac+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--UOx++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--ThAc+++
  .0     .0     .0 0  .0  .0 0 0 0 0 0 0 .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++--ThCit+
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-ThLac+++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-AmOH++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-Am(OH)2+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-PuCO3+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-PuOH++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-Pu(OH)2+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-PuAc++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-PuOx+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-PuLac++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-CaAc+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-CaLac+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-MgAc+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-MgLac+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Mg++-UnuCat#1+

.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-H+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-MgB(OH)4+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-CaB(OH)4+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-Am+++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-AmCO3+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-Th++++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-Pu+++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-NpO2++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-U++++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-UOH+++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-UAc+++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-ThOx++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-AmAc++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-AmLac++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-AmOx+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-UCit+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-ULac+++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-UOx++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-ThAc+++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-ThCit+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-ThLac+++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-AmOH++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-Am(OH)2+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-PuCO3+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-PuOH++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-Pu(OH)2+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-PuAc++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-PuOx+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-PuLac++
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-CaAc+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-CaLac+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-MgAc+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-MgLac+
.0  .0  .0 0  .0  .0  0 0 0 0 0 0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgOH+-UnuCat#1+

 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-MgB(OH)4+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-CaB(OH)4+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-Am+++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-AmCO3+
.37 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-Th++++     Roy92
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-Pu+++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-NpO2++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-U++++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-UOH+++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-UAc+++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-ThOx++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-AmAc++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-AmLac++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-AmOx+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-UCit+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-ULac+++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-UOx++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-ThAc+++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-ThCit+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-ThLac+++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-AmOH++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-Am(OH)2+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-PuCO3+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-PuOH++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-Pu(OH)2+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-PuAc++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-PuOx+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-PuLac++
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-CaAc+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-CaLac+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-MgAc+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-MgLac+
 .0 0 0 0 0 0 0 0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-CaB(OH)4+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-Am+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-AmCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-Th++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-Pu+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-NpO2++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-U++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-UOH+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgB(OH)4+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-Am+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-AmCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-Th++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-Pu+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-NpO2++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-U++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-UOH+++
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaB(OH)4+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-AmCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-Th++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-Pu+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-NpO2++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-U++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-UOH+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am+++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-Th++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-Pu+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-NpO2++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-U++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-UOH+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmCO3+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-Pu+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-NpO2++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-U++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-UOH+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th++++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-NpO2++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-U++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-UOH+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu+++-UCit+
```

```
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu++++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-U++++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-UOH+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-UOH+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 U++++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-UAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOH+++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-ThOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UAc+++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-AmAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-AmOx+
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThOx++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-AmLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmAc++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-AmOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmLac++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-UCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOx+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-ULac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UCit+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-UOx++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ULac+++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-ThAc+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-AmOH++
```

```
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 UOx++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-ThCit+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThAc+++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-ThLac+++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThCit+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-AmOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ThLac+++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-Am(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmOH++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-PuCO3+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(OH)2+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-PuOH++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuCO3+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-Pu(OH)2+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOH++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu(OH)2+-PuAc++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu(OH)2+-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu(OH)2+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu(OH)2+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu(OH)2+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu(OH)2+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu(OH)2+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Pu(OH)2+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuAc++-PuOx+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuAc++-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuAc++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuAc++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuAc++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuAc++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuAc++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOx+-PuLac++
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOx+-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOx+-CaLac+
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOx+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOx+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuOx+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuLac++-CaAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuLac++-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuLac++-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuLac++-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PuLac++-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaAc+-CaLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaAc+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaAc+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaAc+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaLac+-MgAc+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaLac+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CaLac+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgAc+-MgLac+
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgAc+-UnuCat#1+

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 MgLac+-UnuCat#1+



  .0014      .0  -.018  -.004 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- SO4:(vs Cations) psi
  -.006      .0     .0     .0 0 .013 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- HSO4:
  -.006  -.006  -.025     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- OH:
  -.015      .0     .0  -.096 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- HCO3:
  .0085    .004     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- CO3:
 -.0073      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- B(OH)4:
  -.024      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- B3O3(OH)4:
   .026      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- B4O5(OH)4:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Br:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Am(CO3)2:
  .0273      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Am(CO3)3: RRFPH96
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- ClO4-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- NpO2(OH)2-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- NpO2CO3-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- NpO2(CO3)2=-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- NpO2(CO3)3==-:
     .0    -.01     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- H2PO4-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- HPO4=:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- PO4=-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Th(SO4)3=:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Th(OH)3CO3-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Th(CO3)5===:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- HOx-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Ox=            RCM96
 .01029      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Ac-            Mig95
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Lac-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- H2Cit=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- HCit=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Cit=-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- H3EDTA-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- H2EDTA=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- HEDTA=-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- EDTA==
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- AmEDTA=-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- NpO2Cit=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- NpO2EDTA==-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- NpO2Ox-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- U(OH)3CO3-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- U(CO3)5===
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- U(SO4)3=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Pu(CO3)2-
  .0273      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- Pu(CO3)3=-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- PuEDTA-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- CaCit-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- CaEDTA=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- UnuAn#2-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- UnuAn#3-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- UnuAn#4-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- U(OH)2(CO3)2=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- MgCit-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- MgEDTA=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cl- UnuAn#1-

 -.0094  -.0677     .0 -.0425 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= HSO4:
  -.009   -.050     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= OH:
  -.005      .0     .0  -.161 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= HCO3:
  -.005   -.009     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= CO3:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= B(OH)4:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= B3O3(OH)4:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= B4O5(OH)4:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Br:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Am(CO3)2:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Am(CO3)3:
  .0014      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= ClO4-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= NpO2(OH)2-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= NpO2CO3-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= NpO2(CO3)2=-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= NpO2(CO3)3==-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= H2PO4-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= HPO4=:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= PO4=-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Th(SO4)3=:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Th(OH)3CO3-:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Th(CO3)5===:
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= HOx-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Ox=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Ac-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Lac-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= H2Cit=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= HCit=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Cit=-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= H3EDTA-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= H2EDTA=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= HEDTA=-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= EDTA==
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= AmEDTA=-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= NpO2Cit=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= NpO2EDTA==-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= NpO2Ox-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= U(OH)3CO3-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= U(CO3)5===
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= U(SO4)3=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Pu(CO3)2-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= Pu(CO3)3=-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= PuEDTA-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= CaCit-
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= CaEDTA=
     .0      .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4= UnuAn#2-
```

```
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= UnuAn#3-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= UnuAn#4-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= U(OH)2(CO3)2=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= MgCit-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= MgEDTA=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= UnuAn#1-

  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- OH:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HCO3-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- CO3=:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- B(OH)4-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- B3O3(OH)4:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- B4O5(OH)4:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Br-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Am(CO3)2-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Am(CO3)2=-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- ClO4-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2(OH)2-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2CO3-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2(CO3)2=-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2(CO3)3==-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- H2PO4-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HPO4=:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- PO4=-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Th(SO4)3=:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Th(OH)3CO3-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Th(CO3)5===:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HOx-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Ox=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Ac-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Lac-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- H2Cit=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HCit=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Cit=-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- H3EDTA-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- H2EDTA=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HEDTA=-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- EDTA==
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- AmEDTA=-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2Cit=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2EDTA==-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2Ox-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- U(OH)3CO3-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- U(CO3)5===
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- U(SO4)3=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Pu(CO3)2-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Pu(CO3)3=-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- PuEDTA-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- CaCit-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- CaEDTA=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- UnuAn#2-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- UnuAn#3-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- UnuAn#4-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- U(OH)2(CO3)2=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- MgCit-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- MgEDTA=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- UnuAn#1-

  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HCO3:
-.017  -.01    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- CO3:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- B(OH)4:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- B3O3(OH)4:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- B4O5(OH)4:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Br:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Am(CO3)2:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Am(CO3)3:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- ClO4-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2(OH)2-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2CO3-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2(CO3)2=-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2(CO3)3==-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- H2PO4-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HPO4=:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- PO4=-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Th(SO4)3=:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Th(OH)3CO3-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Th(CO3)5===:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HOx-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Ox=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Ac-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Lac-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- H2Cit=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HCit=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Cit=-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- H3EDTA-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- H2EDTA=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HEDTA=-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- EDTA==
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- AmEDTA=-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2Cit=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2EDTA==-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2Ox-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- U(OH)3CO3-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- U(CO3)5===
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- U(SO4)3=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Pu(CO3)2-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Pu(CO3)3=-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- PuEDTA-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- CaCit-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- CaEDTA=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- UnuAn#2-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- UnuAn#3-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- UnuAn#4-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- U(OH)2(CO3)2=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- MgCit-
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- MgEDTA=
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- UnuAn#1-

 .002  .012    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-CO3:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-B(OH)4:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-B3O3(OH)4:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-B4O5(OH)4:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Br:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Am(CO3)2:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Am(CO3)3:
-.010    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-ClO4-:          NPRR95
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2(OH)2-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2CO3-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2(CO3)2=-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2(CO3)3==-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-H2PO4-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-HPO4=:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-PO4=-:
  .0     .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Th(SO4)3=:
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Th(OH)3CO3-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Th(CO3)5===;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-HOx-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Ox=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Ac-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Lac-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-H2Cit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-HCit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Cit=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-H3EDTA-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-H2EDTA=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-HEDTA=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-EDTA==
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-AmEDTA=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2Cit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2EDTA==-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2Ox-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-U(OH)3CO3-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-U(CO3)5===
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-U(SO4)3=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- Pu(CO3)2-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- Pu(CO3)3=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- PuEDTA-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- CaCit-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- CaEDTA=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- UnuAn#2-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- UnuAn#3-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- UnuAn#4-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- U(OH)2(CO3)2=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- MgCit-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- MgEDTA=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- UnuAn#1-

 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= B(OH)4-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= B3O3(OH)4;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= B4O5(OH)4;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Br;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Am(CO3)2;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Am(CO3)3;
-.024  .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= ClO4-;          NPRK95
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2(OH)2-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2CO3-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2(CO3)2=-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2(CO3)3==-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= H2PO4-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= HPO4=;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= PO4=-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Th(SO4)3=;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Th(OH)3CO3-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Th(CO3)5===;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= HOx-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Ox=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Ac-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Lac-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= H2Cit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= HCit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Cit=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= H3EDTA-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= H2EDTA=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= HEDTA=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= EDTA==
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= AmEDTA=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2Cit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2EDTA==-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2Ox-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= U(OH)3CO3-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= U(CO3)5===
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= U(SO4)3=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Pu(CO3)2-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Pu(CO3)3=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= PuEDTA-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= CaCit-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= CaEDTA=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= UnuAn#2-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= UnuAn#3-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= UnuAn#4-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= U(OH)2(CO3)2=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= MgCit-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= MgEDTA=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= UnuAn#1-

 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- B3O3(OH)4;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- B4O5(OH)4;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Br;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Am(CO3)2;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Am(CO3)3;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- ClO4-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2(OH)2-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2CO3-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2(CO3)2=-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2(CO3)3==-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- H2PO4-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- HPO4=;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- PO4=-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Th(SO4)3=;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Th(OH)3CO3-;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Th(CO3)5===;
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- HOx-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Ox=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Ac-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Lac-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- H2Cit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- HCit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Cit=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- H3EDTA-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- H2EDTA=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- HEDTA=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- EDTA==
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- AmEDTA=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2Cit=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2EDTA==-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2Ox-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- U(OH)3CO3-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- U(CO3)5===
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- U(SO4)3=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Pu(CO3)2-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Pu(CO3)3=-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- PuEDTA-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- CaCit-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- CaEDTA=
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- UnuAn#2-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- UnuAn#3-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- UnuAn#4-
 .0    .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- U(OH)2(CO3)2=
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- B4O5(OH)4;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Br;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Am(CO3)2;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Am(CO3)3;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- ClO4-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2(OH)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2CO3-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2(CO3)2=-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2(CO3)3==-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- H2PO4-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- HPO4=;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- PO4=-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Th(SO4)3=;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Th(OH)3CO3-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Th(CO3)5===;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- HOx-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Ox=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Ac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Lac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- H2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- HCit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Cit=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- H3EDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- H2EDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- HEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- EDTA==
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- AmEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Br;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Am(CO3)2;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Am(CO3)3;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= ClO4-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NPO2(OH)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2CO3-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2(CO3)2=-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2(CO3)3==-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= H2PO4-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= HPO4=;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= PO4=-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Th(SO4)3=;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Th(OH)3CO3-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Th(CO3)5===;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= HOx-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Ox=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Ac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Lac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= H2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= HCit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Cit=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= H3EDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= H2EDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= HEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= EDTA==
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= AmEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Am(CO3)2;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Am(CO3)3;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- ClO4-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2(OH)2-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2CO3-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2(CO3)2=-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2(CO3)3==-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- H2PO4-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- HPO4=;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- PO4=-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Th(SO4)3=;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Th(OH)3CO3-;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Th(CO3)5===;
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- HOx-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Ox=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Ac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Lac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- H2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- HCit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Cit=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- H3EDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- H2EDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- HEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- EDTA==
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- AmEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- U(OH)3CO3-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	U(CO3)5===	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	U(SO4)3=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	Pu(CO3)2-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	Pu(CO3)3=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	PuEDTA-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	CaCit-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	CaEDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	UnuAn#2-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	UnuAn#3-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	UnuAn#4-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	U(OH)2(CO3)2=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	MgCit-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	MgEDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Br-	UnuAn#1-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Am(CO3)3;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	ClO4-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	NpO2(OH)2-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	NpO2CO3-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	NpO2(CO3)2=-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	NpO2(CO3)3==-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	H2PO4-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	HPO4=;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	PO4=-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Th(SO4)3=;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Th(OH)3CO3-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Th(CO3)5===;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	HOx-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Ox=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Ac-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Lac-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	H2Cit=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	HCit=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Cit=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	H3EDTA-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	H2EDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	HEDTA=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	EDTA==	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	AmEDTA=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	NpO2Cit=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	NpO2EDTA==-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	NpO2Ox-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	U(OH)3CO3-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	U(CO3)5===	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	U(SO4)3=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Pu(CO3)2-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	Pu(CO3)3=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	PuEDTA-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	CaCit-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	CaEDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	UnuAn#2-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	UnuAn#3-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	UnuAn#4-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	U(OH)2(CO3)2=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	MgCit-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	MgEDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)2-	UnuAn#1-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	ClO4-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	NpO2(OH)2-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	NpO2CO3-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	NpO2(CO3)2=-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	NpO2(CO3)3==-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	H2PO4-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	HPO4=;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	PO4=-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Th(SO4)3=;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Th(OH)3CO3-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Th(CO3)5===;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	HOx-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Ox=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Ac-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Lac-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	H2Cit=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	HCit=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Cit=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	H3EDTA-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	H2EDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	HEDTA=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	EDTA==	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	AmEDTA=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	NpO2Cit=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	NpO2EDTA==-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	NpO2Ox-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	U(OH)3CO3-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	U(CO3)5===	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	U(SO4)3=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Pu(CO3)2-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	Pu(CO3)3=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	PuEDTA-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	CaCit-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	CaEDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	UnuAn#2-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	UnuAn#3-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	UnuAn#4-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	U(OH)2(CO3)2=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	MgCit-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	MgEDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Am(CO3)3=-	UnuAn#1-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	NpO2(OH)2-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	NpO2CO3-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	NpO2(CO3)2=-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	NpO2(CO3)3==-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	H2PO4-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	HPO4=;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	PO4=-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	Th(SO4)3=;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	Th(OH)3CO3-;	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	Th(CO3)5===;	
-.0814	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	HOx-	RCM96
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	Ox=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	Ac-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	Lac-	
.0162	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	H2Cit=	RCM96
.0213	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	HCit=	RCM96
.019	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	Cit=-	RCM96
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	H3EDTA-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	H2EDTA=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	HEDTA=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	EDTA==	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	AmEDTA=-	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	NpO2Cit=	
.0	.0	.0	.0 0	.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ClO4-	NpO2EDTA==-	

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- NpO2Ox-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- U(OH)3CO3-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- U(CO3)5===
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- U(SO4)3=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- Pu(CO3)2-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- Pu(CO3)3=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- PuEDTA-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- CaCit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- CaEDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- UnuAn#2-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- UnuAn#3-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- UnuAn#4-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- U(OH)2(CO3)2=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- MgCit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- MgEDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4- UnuAn#1-

.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- NpO2CO3-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- NpO2(CO3)2=-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- NpO2(CO3)3==-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- H2PO4-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- HPO4=:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- PO4=-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Th(SO4)3=:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Th(OH)3CO3-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Th(CO3)5===:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- HOx-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Ox=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Ac-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Lac-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- H2Cit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- HCit=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Cit=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- H3EDTA-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- H2EDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- HEDTA=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- EDTA==
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- AmEDTA=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- NpO2Cit=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- NpO2EDTA==-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- NpO2Ox-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- U(OH)3CO3-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- U(CO3)5===
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- U(SO4)3=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Pu(CO3)2-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- Pu(CO3)3=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- PuEDTA-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- CaCit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- CaEDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- UnuAn#2-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- UnuAn#3-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- UnuAn#4-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- U(OH)2(CO3)2=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- MgCit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- MgEDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2- UnuAn#1-

.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- NpO2(CO3)2=-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- NpO2(CO3)3==-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- H2PO4-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- HPO4=:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- PO4=-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Th(SO4)3=:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Th(OH)3CO3-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Th(CO3)5===:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- HOx-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Ox=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Ac-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Lac-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- H2Cit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- HCit=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Cit=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- H3EDTA-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- H2EDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- HEDTA=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- EDTA==
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- AmEDTA=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- NpO2Cit=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- NpO2EDTA==-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- NpO2Ox-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- U(OH)3CO3-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- U(CO3)5===
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- U(SO4)3=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Pu(CO3)2-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- Pu(CO3)3=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- PuEDTA-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- CaCit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- CaEDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- UnuAn#2-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- UnuAn#3-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- UnuAn#4-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- U(OH)2(CO3)2=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- MgCit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- MgEDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2CO3- UnuAn#1-

.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- NpO2(CO3)3==-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- H2PO4-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- HPO4=:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- PO4=-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Th(SO4)3=:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Th(OH)3CO3-:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Th(CO3)5===:
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- HOx-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Ox=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Ac-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Lac-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- H2Cit-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- HCit=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Cit=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- H3EDTA-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- H2EDTA=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- HEDTA=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- EDTA==
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- AmEDTA=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- NpO2Cit=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- NpO2EDTA==-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- NpO2Ox-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- U(OH)3CO3-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- U(CO3)5===
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- U(SO4)3=
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Pu(CO3)2-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- Pu(CO3)3=-
.0 .0 .0 .0 0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(CO3)2=- PuEDTA-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- UnuAn#2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- U(OH)2(CO3)2=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- MgCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- MgEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- UnuAn#1-

 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- H2PO4-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- HPO4=:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- PO4=-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Th(SO4)3=:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Th(OH)3CO3-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Th(CO3)5===:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- HOx-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Ox=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Ac-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Lac-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- H2Cit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- HCit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Cit=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- H3EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- H2EDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- HEDTA=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- EDTA==
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- AmEDTA=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- NpO2Cit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- NpO2EDTA==-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- NpO2Ox-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- U(OH)3CO3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- U(CO3)5===
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- U(SO4)3=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Pu(CO3)2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Pu(CO3)3=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- PuEDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- UnuAn#2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- U(OH)2(CO3)2=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- MgCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- MgEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- UnuAn#1-

 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- HPO4=:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- PO4=-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Th(SO4)3=:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Th(OH)3CO3-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Th(CO3)5===:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- HOx-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Ox=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Ac-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Lac-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- H2Cit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- HCit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Cit=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- H3EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- H2EDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- HEDTA=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- EDTA==
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- AmEDTA=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- NpO2Cit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- NpO2EDTA==-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- NpO2Ox-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- U(OH)3CO3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- U(CO3)5===
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- U(SO4)3=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Pu(CO3)2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Pu(CO3)3=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- PuEDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- UnuAn#2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- U(OH)2(CO3)2=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- MgCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- MgEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- UnuAn#1-

 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= PO4=-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Th(SO4)3=:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Th(OH)3CO3-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Th(CO3)5===:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= HOx-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Ox=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Ac-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Lac-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= H2Cit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= HCit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Cit=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= H3EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= H2EDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= HEDTA=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= EDTA==
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= AmEDTA=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= NpO2Cit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= NpO2EDTA==-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= NpO2Ox-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= U(OH)3CO3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= U(CO3)5===
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= U(SO4)3=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Pu(CO3)2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= Pu(CO3)3=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= PuEDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= UnuAn#2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= U(OH)2(CO3)2=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= MgCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= MgEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HPO4= UnuAn#1-

 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=- Th(SO4)3=:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=- Th(OH)3CO3-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=- Th(CO3)5===:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=- HOx-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=- Ox=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=- Ac-
```

```
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- Lac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- H2Cit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- HCit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- Cit=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- NpO2EDTA==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=- UnuAn#1-

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= Th(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= Th(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= HOx-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= Ox=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= Ac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= Lac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= H2Cit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= HCit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= Cit=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= NpO2EDTA==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)3= UnuAn#1-

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- Th(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- HOx-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- Ox=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- Ac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- Lac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- H2Cit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- HCit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- Cit=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- NpO2EDTA==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)3CO3- UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)4CO3- U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)4CO3- MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)4CO3- MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)4CO3- UnuAn#1-

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== HOx-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== Ox=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== Ac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== Lac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== H2Cit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== HCit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== Cit=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== NpO2EDTA==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(CO3)5=== UnuAn#1-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- Ox=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- Ac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- Lac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- H2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- HCit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- Cit=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- H3EDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- H2EDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- HEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- EDTA==
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- AmEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= Ac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= Lac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= H2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= HCit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= Cit=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= H3EDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= H2EDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= HEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= EDTA==
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= AmEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox= UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- Lac-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- H2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- HCit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- Cit=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- H3EDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- H2EDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- HEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- EDTA==
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- AmEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- H2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- HCit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- Cit=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- H3EDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- H2EDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- HEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- EDTA==
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- AmEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- HCit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- Cit=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- H3EDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- H2EDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- HEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- EDTA==
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- AmEDTA=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit- NpO2Ox-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Cit- UnuAn#1-

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= Cit=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= NpO2EDTA---
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= UnuAn#1-

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- NpO2EDTA---
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- UnuAn#1-

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- NpO2EDTA---
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- UnuAn#1-

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= NpO2EDTA---
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= UnuAn#1-

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- AmEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- NpO2EDTA---
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- Pu(CO3)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- Pu(CO3)3=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- PuEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- UnuAn#2-
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== AmEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- NpO2Cit=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= NpO2EDTA==-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- NpO2Ox-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA==- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- U(OH)3CO3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3-U(CO3)5===
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3-U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- MgEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- UnuAn#1-

.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== U(SO4)3=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== Pu(CO3)2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== Pu(CO3)3=-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== PuEDTA-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== CaCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== CaEDTA=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== UnuAn#2-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== UnuAn#3-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== UnuAn#4-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== U(OH)2(CO3)2=
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== MgCit-
.0  .0  .0  .0 0  .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== MgEDTA=
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5==== UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= Pu(CO3)2-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= Pu(CO3)3=-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= PuEDTA-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= CaCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= CaEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= UnuAn#2-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= UnuAn#3-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= UnuAn#4-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- Pu(CO3)3=-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- PuEDTA-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- CaCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- CaEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- UnuAn#2-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- UnuAn#3-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- UnuAn#4-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)2- UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- PuEDTA-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- CaCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- CaEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- UnuAn#2-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- UnuAn#3-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- UnuAn#4-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(CO3)3=- UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- CaCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- CaEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- UnuAn#2-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- UnuAn#3-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- UnuAn#4-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuEDTA- UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- CaEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- UnuAn#2-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- UnuAn#3-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- UnuAn#4-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= UnuAn#2-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= UnuAn#3-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= UnuAn#4-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- UnuAn#3-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- UnuAn#4-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- UnuAn#4-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#4- U(OH)2(CO3)2=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#4- MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#4- MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#4- UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)2(CO3)2= MgCit-
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)2(CO3)2= MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)2(CO3)2= UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgCit- MgEDTA=
 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgCit- UnuAn#1-

 .0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgEDTA= UnuAn#1-

 .100 .051  .183 .183 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO2-Cations        HMW84 lambda
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCO3-Cations      HMW84
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgCO3-Cations      HMW84
-.097 -.14  .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)3-Cations     FW86
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2OH-Cations
  .0 -.07   .0   .0 .0  .29   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3PO4-Cations      PS76
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)2-Cations
  .0   .0   .0   .0 .0  .524  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Ox-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(OH)3(aq)-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HAc-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ac-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HLac-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3Citrate-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmCit-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Lac-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)4-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)4-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)2-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(OH)3(aq)-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuCit(aq)-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaOx(aq)-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H4EDTA-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ThEDTA-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UEDTA-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgOx(aq)-Cations
  .0   .0   .0   .0 .0  .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuNeu#1-Cations

-.005 .097 -.003  0 0 0 0  .0 0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO2-An       HMW84
  .0   .0   .0    0 0 0 0  .0 0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCO3-An     HMW84
  .0   .0   .0    0 0 0 0  .0 0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgCO3-An     HMW84
 .091 .018  .0    0 0 0 0 -.2 0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)3-An    FW86
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
  -.19    .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2OH-An    FHR95
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0 -.4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3PO4-An     PS76
   .29    .0  .68   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)2-An Roy92
  .035    .0  .126  0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Ox-An
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  An(OH)3(aq)-An
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HAc-An
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ac-An
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HLac-An
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3Citrate-An
-.2731    .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmCit-An     RCM96
-.1853    .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Lac-An   RCM96
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)4-An
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)4-An
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)2-An
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Pu(OH)3(aq)-An
-.2731    .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PuCit(aq)-An
 -.00514  .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaOx(aq)-An     RCM96
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H4EDTA-An
 -.832    .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ThEDTA-An    RCM96
 -.832    .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UEDTA-An
 -.00514  .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgOx(aq)-An    RCM96
   .0     .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuNeu#1-An

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   CO2-C-A
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0    (C down
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0     A acr
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   CaCO3-Cation-Anion
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   MgCO3-Cation-Anion
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .046 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)3-Cation-Anion FW86
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   (Cat down. Anions across)
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-.0102 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   NpO2OH-C-A
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H3PO4-Cation-Anion
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)2-Cation-Anion
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Ox-Cation-Anion
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(OH)3(aq)-Cation-Anion
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HAc-Cation-Anion
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2Ac-Cation-Anion
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HLac-Cation-Anion
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
5205  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5206  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5207  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5208  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5209  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5210  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5211
5212  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H3Cit-Cation-Anion
5213  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5214  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5215  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5216  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5217  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5218  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5219  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5220  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5221  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5222  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5223  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5224  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5225  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5226  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5227  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5228  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5229  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5230  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5231  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5232  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5233  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5234  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5235  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5236  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5237  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5238  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5239  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5240  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5241  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5242  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5243  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5244  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5245  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5246  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5247  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5248  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5249  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5250  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5251
5252  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   AmCit-Cation-Anion
5253  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5254  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5255  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5256  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5257  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5258  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5259  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5260  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5261  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5262  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5263  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5264  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5265  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5266  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5267  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5268  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5269  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5270  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5271  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5272  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5273  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5274  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5275  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5276  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5277  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5278  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5279  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5280  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5281  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5282  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5283  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5284  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5285  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5286  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5287  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5288  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5289  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5290  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5291
5292  .059 .0 .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   NpO2Lac-Cation-Anion
5293  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5294  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5295  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5296  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5297  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5298  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5299  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5300  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5301  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5302  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5303  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5304  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5305  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5306  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5307  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5308  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5309  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5310  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5311  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5312  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5313  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5314  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5315  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5316  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5317  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5318  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5319  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5320  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5321  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5322  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5323  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5324  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5325  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5326  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5327  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5328  .0  .0  .0  .0  .0  .0  0 0 0 0 0 0 0 0 0 0 0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)4-Cation-Anion
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   U(OH)4-Cation-Anion
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   U(SO4)2-Cation-Anion
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Pu(OH)3(aq)-Cation-Anion
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PuCit(aq)-Cation-Anion
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   CaOx(aq)-Cation-Anion
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H4EDTA-C-A
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   ThEDTA-C-A
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   UEDTA-C-A
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0


.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   MgOx(aq)-C-A
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0


.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuNeu#1-C-A
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.0 .0 .0 .0 .0 .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

  2   3   4   5   6   7    Na+          K+           Ca++         Mg++         MgOH+   H+              cation map ELMAP(1,)
 22  21  36  37  50  43    MgB(OH)4+ CaB(OH)4+ Am+++       AmCO3+       Th++++ Pu+++
 64  56  57 101  99  86    NpO2+        U++++        UOH+++       UAc+++       ThOx++ AmAc++
 90  89 102 104 105  96    AmLac++      AmOx+        UCit+        ULac+++      UOx++  ThAc+++
 97 100  40  41  44  47    ThCit+       ThLac+++     AmOH++       Am(OH)2+ PuCO3+ PuOH++
 48  91  94  95 116 120    Pu(OH)2+     PuAc++       PuOx+        PuLac++      CaAc+  CaLac+
111 115 121                MgAc+        MgLac+       UnuCat#1+

  8   9  10  11  12  13    Cl-          SO4=         HSO4-          OH-              HCO3-          CO3=          anion map ELMAP(2,)
 18  19  20  23  38  39    B(OH)4-      B3O3(OH)4-   B4O5(OH)4=     Br-              Am(CO3)2-      Am(CO3)3=-
 24  69  65  66  67  33    ClO4-        NpO2(OH)2-   NpO2CO3-       NpO2(CO3)2=-     NpO2(CO3)3==-  H2PO4-
 34  35  55  52  51  82    HPO4=        PO4=-        Th(SO4)3=      Th(OH)3(CO3)-    Th(CO3)5===    HOx-
 83  71  85  73  74  75    Ox=          Ac-          Lac-           H2Cit-           HCit=          Cit=-
 77  78  79  80  88 107    H3EDTA-      H2EDTA=      HEDTA=-        EDTA==           AmEDTA=-       NpO2Cit=
108 109  60  58  63  45    NpO2EDTA=-   NpO2Ox-      U(OH)4(CO3)2== U(CO3)5===       U(SO4)3=       Pu(CO3)2-
 46  93 117 118 123 124    Pu(CO3)3=-   PuEDTA-      CaCit-         CaEDTA=          UnuAn#2-       UnuAn#3-
125  59 112 113 122        UnuAn#4-     U(OH)2(CO3)2= MgCit-        MgEDTA=          UnuAn#1-

 14  15  16  17  68  32    CO2          CaCO3        MgCO3          B(OH)3  NpO2OH H3PO4      neutral map ELMAP(3,)
 54  81  42  70 106  84    Th(SO4)2     H2Ox         Am(OH)3(aq)    HAc     NpO2Ac HLac
 72  87 110  53  61  62    H3Cit        AmCit        NpO2Lac        Th(OH)4 U(OH)4 U(SO4)2
 49  92 119  76  98 103    Pu(OH)3(aq)  PuCit(aq)    CaOx(aq)       H4EDTA  ThEDTA UEDTA
116 126                    MgOx(aq)     UnuNeu#1

'nEQUALACT' 0

2 (Oxygen)
'nREDOX' 0
'nIONEX' 0 0 'nMF'

123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012
         1         2         3         4         5         6         7         8         9         0         1         2         3
                                                                                                   1         1         1         1

Data values without explicit references are from HMW84 or FW86

+III References
 FRSR89 ==  Felmy, Rai, Schramke, and Ryan (1989) RCA 48 pp.29-35
 FRF90  ==  Felmy, Rai, and Fulton (1990) RCA 50 pp.193-204
 RFF92  ==  Rai, Felmy, and Fulton (1992)  RCA 56 pp.7-14
 RFFR92 ==  Rai, Felmy, Fulton, and Ryan (1992) RCA 58/59 pp.9-16
 RFF94  ==  Rai, Felmy, and Fulton (1994)
 RRFFN96 ==  Rao, Rai, Felmy, Fulton, and Novak, for RCA
 CFN11JUN96 =  Novak 11Jun96 memo "Parameter Values for +III Actinide Hydrolysis Species"
 FKPKH94 ==  Fanghanel, Kim, et al.  RCA 66/67 81-87 "Thermo of Radioactive Trace Elements in
             Conc Electrolyte Solutions:  Hydrolysis of Cm+++ in NaCl Solutions"

+IV References
 FRM91  ==  Felmy, Rai, and Mason (1991) RCA 55 pp.177-185
 FR92   ==  Felmy and Rai (1992) J Soln Chem 21#5 pp.407-423
 Roy92  ==  Roy et al (1992) J Phys Chem 96#26 pp.11065-11072
 Rai96  ==  U(IV) Fax from Dhan Rai, 13 Mar 96
```

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

```
5825    RFSM90N **  Rai et al. 1996  Solubility of Th(IV) and U(IV) Hydrous Oxides in Conc NaCl and MgCl2 Solutions
5826    FREMHC96 ** Felmy,Rai,Sterner,Mason,Hess,Conradson "Thermo Models for Highly Charged Aq Species
5827                Solubility of Th(IV) Hydrous Oxide in Conc NaHCO3 and Na2CO3 Solns"
5828
5829    *V References
5830     NR94    **  Novak and Roberts (1994) SAND94-0805C MRS/Kyoto
5831     FNK95   **  Fanghanel et al.  (1995) RCA 6983 pp.169-176 "Thermo of Np(V):  IIP's for Hydrolysis and Carbonate Complexes"
5832     N95     **  Novak 1995 memo of 1 OCT 95
5833     LBL95   **  Novak memo analyzing Np(V)/K2CO3 Experiments, 17OCT95
5834
5835    Organic Ligand References
5836     CFN950705 **  Novak memo to EJNowaX
5837     RCM96     **  RC Moore, 22FEB96 memorandum "Final Model Parameters for Deprotponation of..."
5838     RCM96b    **  RC Moore, 14Mar96 memo "Revision 1.  Final Model Parameters..."
5839     RCM96c    **  RC Moore, 17Mar96 memo "Model Parameters for Magnesium Complexation..."
5840     NBC96     **  Novak, Borkowski, Choppin RCA (1996)  "Thermo Modling of Np(V)-Acetate...in Conc NaCl"
5841     CFN16APR96 *  Novak 16Apr96 memo "Thermo Parms fo the Solubility of <<oxalate solids>>"
5842
5843    General References
5844     HMW84   **  Harvie, Moller, Weare (1984) GCA 48 pp.723-751
5845     FW86    **  Felmy and Weare (1986) GCA 50 pp.2771-2783
5846     PS76    **  Pitzer and Silvester (1976) J Soln Chem 5#4 pp.269-278
5847     P91     **  Pitzer (1991) CRC Handbook, Activity Coef in Electrolyte Solns
5848     CFN95a  **  Novak (1995a) 18Jan95 Memo "Creation and Definition of the Database for FMT called "HMW_NP_AM.CHEMDAT..."
5849     NFRK95  **  Neck et al. (1995) RCA 6981 pp. 39-47, "Thermo of Np(V) in Conc Salt Solns..."
5850
```

Appendix X: Current Data Base, HMW_Am3Pu3Th4Np5_960823.RHOMIN

```
1     2000.0
2     2000.0
3     2000.0
4     2000.0
5     2000.0
6     2000.0
7     2000.0
8     2000.0
9     2000.0
10    2000.0
11    2000.0
12    2000.0
13    2000.0
14    2000.0
15    2000.0
16    2000.0
17    2000.0
18    2000.0
19    2000.0
20    2000.0
21    2000.0
22    2000.0
23    2000.0
24    2000.0
25    2000.0
26    2000.0
27    2000.0
28    2000.0
29    2000.0
30    2000.0
31    2000.0
32    2000.0
33    2000.0
34    2000.0
35    2000.0
36    2000.0
37    2000.0
38    2000.0
39    2000.0
40    2000.0
41    2000.0
42    2000.0
43    2000.0
44    2000.0
45    2000.0
46    2000.0
47    2000.0
48    2000.0
49    2000.0
50    2000.0
51    2000.0
52    2000.0
53    2000.0
54    2000.0
55    2000.0
56    2000.0
57    2000.0
58    2000.0
59    2000.0
60    2000.0
61    2000.0
62    2000.0
63    2000.0
64    2000.0
65    2000.0
66    2000.0
67    2000.0
68    2000.0
69    2000.0
70    2000.0
71    2000.0
72    2000.0
73    2000.0
74    2000.0
75    2000.0
76    2000.0
77    2000.0
78    2000.0
79    2000.0
80    2000.0
81    2000.0
82    2000.0
83    2000.0
84    2000.0
85
86
```

Appendix Y: Review Forms

This Appendix contains the review forms for the FMT User's Manual.