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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

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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-SO₄-OH-HCO₃-CO₃-CO₂-B-H₂O 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.

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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, MgCl₂, Na₂CO₃, NaHCO₃, K₂CO₃, 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 $\text{CO}_2(\text{g})$ 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

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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).

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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.,

$$\frac{\partial G}{\partial \bar{\xi}} = 0 \quad (1)$$

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

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

where

\mathbf{N}^T = the complete, transposed stoichiometric matrix: the $(N \times R)$ matrix whose columns are the R stoichiometric vectors; that is, $\mathbf{N} = (\bar{v}_1, \bar{v}_2, \dots, \bar{v}_R)$; entry (j) of \mathbf{N} is v_{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 $\delta \bar{\xi}$:

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

where

m = iteration index,

v_{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

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

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

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

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 ($\partial^2 G / \partial \bar{\xi}^2$) for which, in the case of a single ideal phase, can be expressed as

$$\begin{aligned} \frac{\partial^2 G}{\partial \bar{\xi}_i \partial \bar{\xi}_j} &= \frac{\partial}{\partial \bar{\xi}_j} \left(\sum_{k=1}^{N'} v_{ki} \mu_k \right) \\ &= RT \sum_{k=1}^{N'} \sum_{l=1}^{N'} v_{ki} v_{lj} \left(\frac{\delta_{kl}}{n_k} - \frac{1}{n_t} \right); \quad j=1,2,\dots,R, \end{aligned} \quad (6)$$

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

$$RT \left(\frac{\partial^2 G}{\partial \bar{\xi}_i \partial \bar{\xi}_j} \right)^{-1} \approx \left(\frac{1}{n_{i+M}} + \sum_{k=1}^M \frac{v_{ki}^2}{n_k} - \frac{\bar{v}_i^2}{n_t} \right)^{-1} \delta_{ij}, \quad (7)$$

where \bar{v}_i is the sum of the stoichiometric coefficients in stoichiometric equation i ; i.e.

$$\bar{v}_i = \sum_{k=1}^{N'} v_{ki}$$

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

$$\delta \bar{\xi}_j^{(m)} = - \left(\frac{1}{n_{j+M}^{(m)}} + \sum_{k=1}^M \frac{v_{kj}^2}{n_k^{(m)}} - \frac{\bar{v}_j^2}{n_t} \right)^{-1} \frac{\Delta G_j^{(m)}}{RT}; \quad j=1,2,\dots,R. \quad (8)$$

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 through 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:

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

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.

$$a_i = \gamma_i m_i \quad (\text{A.1b})$$

and, for the solvent, by

$$\ln a_{\text{H}_2\text{O}} = \frac{-W}{1000} \left(\sum_i m_i \right) \phi \quad (\text{A.1c})$$

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:

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

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.)

$$\begin{aligned}
 (\phi-1) \frac{\left(\sum_i m_i\right)}{2} = & -\frac{A^\phi I^{3/2}}{1+bl^{1/2}} + \sum_c \sum_a m_c m_a (B_{ca}^\phi + ZC_{ca}) + \sum_c \sum_{c'} m_c m_{c'} \left(\Phi_{cc'}^\phi + \sum_a m_a \Psi_{cc'a} \right) \\
 & + \sum_a \sum_{a'} m_a m_{a'} \left(\Phi_{aa'}^\phi + \sum_c m_c \Psi_{aa'c} \right) + \sum_n \sum_c m_n m_c \lambda_{nc} \\
 & + \sum_n \sum_a m_n m_a \lambda_{na} + \sum_n \sum_c \sum_a m_n m_c m_a \zeta_{nca}
 \end{aligned} \tag{A.2a}$$

$$\begin{aligned}
 \ln \gamma_M = & z_M^2 F + \sum_a m_a (2B_{Ma} + ZC_{Ma}) + \sum_c m_c \left(2\Phi_{Mc} + \sum_a m_a \Psi_{Mca} \right) \\
 & + \sum_a \sum_{a'} m_a m_{a'} \Psi_{aa'M} + |z_M| \left[\sum_c \sum_a m_c m_a C_{ca} + \sum_n m_n (2\lambda_{nM}) + \sum_n \sum_a m_n m_a \zeta_{naM} \right]
 \end{aligned} \tag{A.2b}$$

$$\begin{aligned}
 \ln \gamma_X = & z_X^2 F + \sum_c m_c (2B_{Xc} + ZC_{Xc}) + \sum_a m_a \left(2\Phi_{Xa} + \sum_c m_c \Psi_{Xca} \right) \\
 & + \sum_c \sum_{c'} m_c m_{c'} \Psi_{cc'X} + |z_X| \left[\sum_c \sum_a m_c m_a C_{ca} + \sum_n m_n (2\lambda_{nX}) + \sum_n \sum_c m_n m_c \zeta_{ncX} \right]
 \end{aligned} \tag{A.2c}$$

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

$$\begin{aligned}
 F = & -A^\phi \left(\frac{I^{1/2}}{1+bl^{1/2}} + \frac{2}{b} \ln(1+bl^{1/2}) \right) + \sum_c \sum_a m_c m_a B_{ca} \\
 & + \sum_c \sum_{c'} m_c m_{c'} \Phi_{cc'}^\phi + \sum_a \sum_{a'} m_a m_{a'} \Phi_{aa'}^\phi
 \end{aligned} \tag{A.2e}$$

$$C_{MX} = \frac{C_{MX}^\phi}{2|Z_M Z_X|^{1/2}} \quad (2b)$$

$$Z = \sum_i |z_i| m_i \quad (2c)$$

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

$$\ln \gamma_i^{DH} = -\frac{A\sqrt{I}}{1 + B a_i \sqrt{I}} + B_i I,$$

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:

$$B_{MX}^\phi = \beta_{MX}^{(0)} + \beta_{MX}^{(1)} e^{-\alpha_1 \sqrt{I}} + \beta_{MX}^{(2)} e^{-\alpha_2 \sqrt{I}} \quad (3a)$$

$$B_{MX} = \beta_{MX}^{(0)} + \beta_{MX}^{(1)} g(\alpha_1 \sqrt{I}) + \beta_{MX}^{(2)} g(\alpha_2 \sqrt{I}) \quad (3b)$$

$$B'_{MX} = \beta_{MX}^{(1)} \frac{g'(\alpha_1 \sqrt{I})}{I} + \beta_{MX}^{(2)} \frac{g'(\alpha_2 \sqrt{I})}{I} \quad (3c)$$

The functions g and g' are defined by

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

INFORMATION ONLY

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

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 electrolytes, $b = 1.2$. For 2 - 3 and higher pairs, $\alpha_1 = 1.4$ and $\alpha_2 = 50$. The dimensions of α_1 and α_2 are $\text{kg}^{1/2} \text{mole}^{-1/2}$. The virial coefficients, Φ , which depend upon ionic strength, are given the following form:

$$\Phi_{ij}^\phi = \theta_{ij} + {}^E\theta_{ij}(I) + I {}^E\theta'_{ij}(I) \quad (5a)$$

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

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

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_{MX}^ϕ 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:

- $\beta_{MX}^{(0)}$, $\beta_{MX}^{(1)}$, $\beta_{MX}^{(2)}$, and C_{MX}^ϕ 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:

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

and

$$\lim_{x_i \rightarrow 1} \gamma_i = 1 \quad (\text{Raoult convention})$$

or

$$\lim_{x_i \rightarrow 0} \gamma_i = 1 \quad (\text{Henry convention})$$

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

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

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

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

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

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

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 $-\text{toll} < \text{computed charge} < +\text{toll}$. 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 $-10^{-6} < \text{computed charge} < 10^{-6}$. 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.

INFORMATION ONLY

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)," "ClO₄," "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 CO₂ gas present. It is therefore desirable to calculate the effects of CO₂ 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 CO₂ gas fugacity by proper declaration of a CO₂ solid phase, as discussed below.

Thermodynamics allows the declaration of a hypothetical CO₂ "solid" phase to mimic the effects of constant CO₂ gas fugacity:



At equilibrium, this reaction is described by the relationship

$$\frac{\mu_{\text{CO}_2(\text{"solid"})}^0}{RT} = \frac{\mu_{\text{CO}_2(g)}^0}{RT} + \ln f_{\text{CO}_2}, \quad (14)$$

where f_{CO_2} is the $\text{CO}_2(g)$ fugacity, which can be thought of as an effective partial pressure for $\text{CO}_2(g)$. 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 $\text{CO}_2(g)$ 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.

INFORMATION ONLY

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.

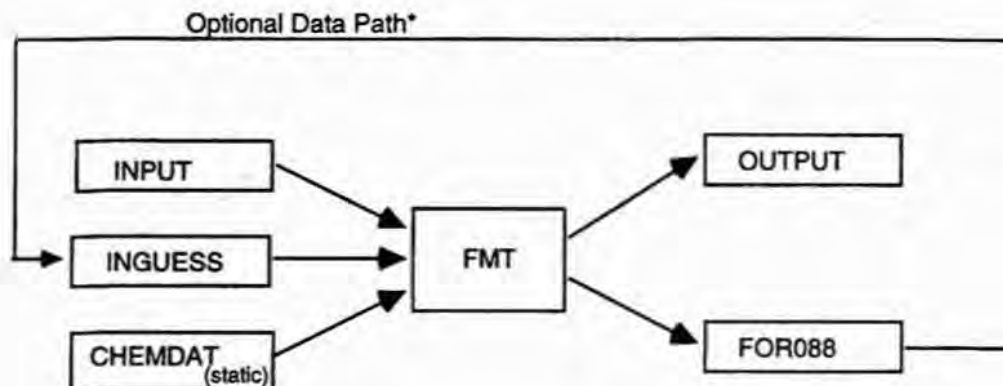
Note that "abundance" means the total amount, an extrinsic quantity, e.g., 3 moles of Na, 2 moles of Cl, 1 mole of Br. The intrinsic quantity, commonly moles per kg H₂O within FMT, is calculated based on the extrinsic amount of water that can be formed from the specified element abundances. This is the 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 H₂O 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 H₂O" 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.



*FOR088 output may be used as input for INGUESS file.

Figure 1. Input and Output Files for BATCH

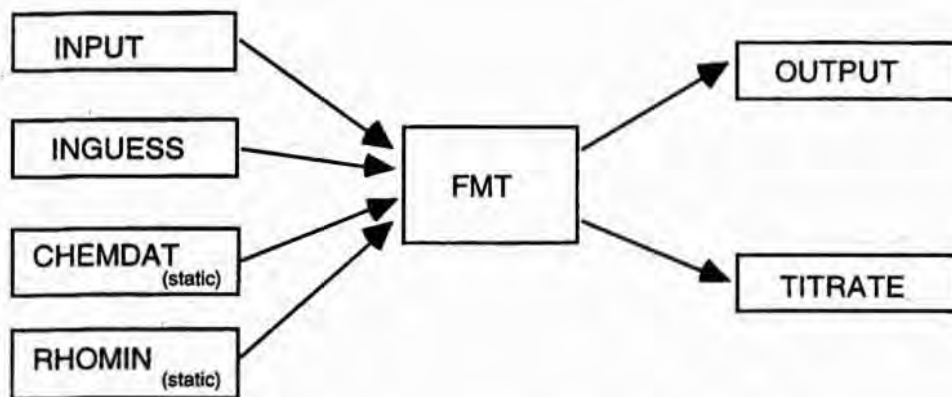


Figure 2. Input and Output Files for TITRATE

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 H₂O. 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.

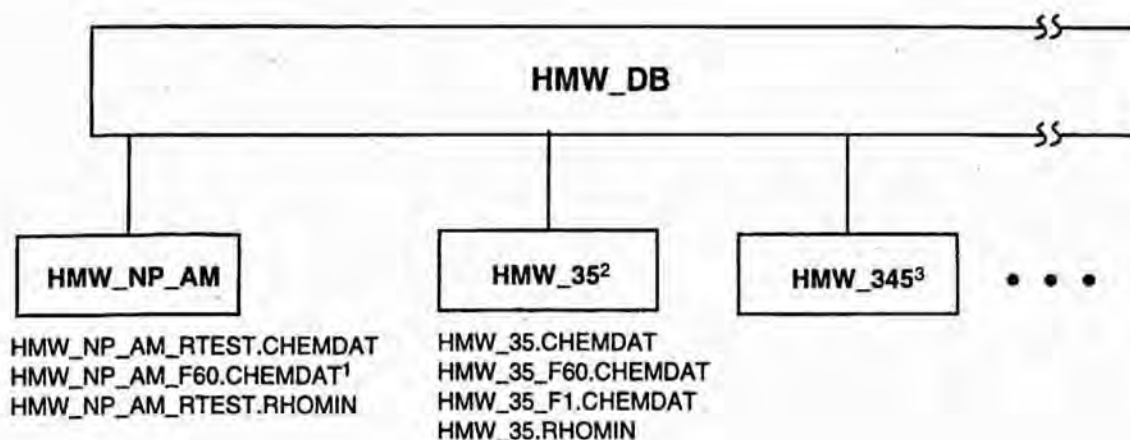
FMT reads the entire INPUT file. If the character strings 'MOLES' and 'EXACT' are set in the INPUT file, then FMT reads the moles for each species from the INGUESS file and calculates the molal amounts of all the elements. If 'nMOLES' and 'nEXACT' strings are set, then FMT uses the elemental mole amounts 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 CO₂ "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 CO₂ "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.

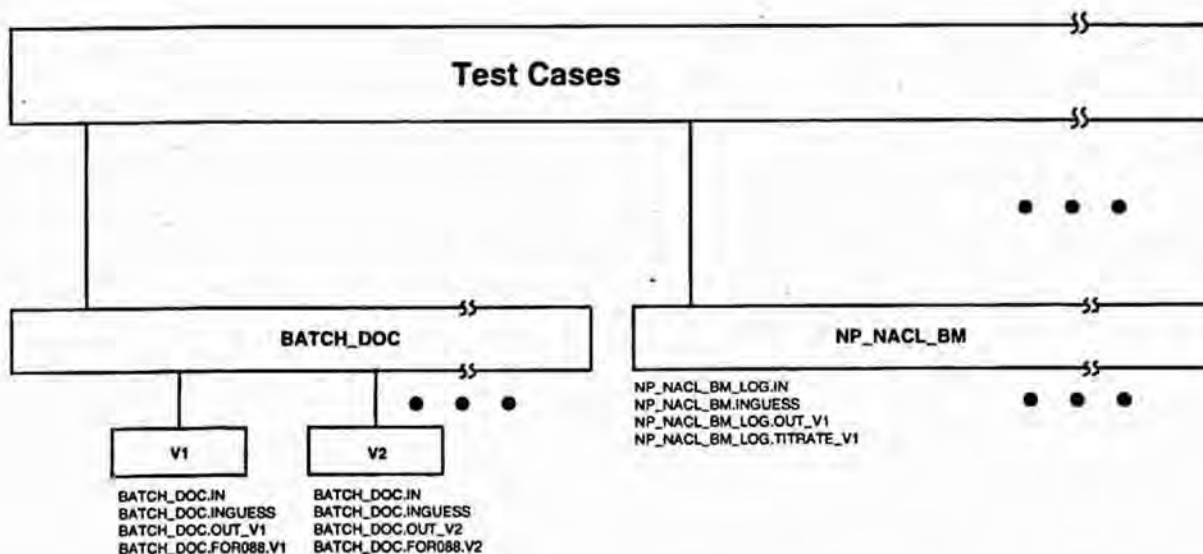


Figure 4. Suggested input/output file organization.

- the output 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: "All-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
```



```
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 identification: " "
        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,RFFF94)

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 2.171E-07 -6.66
fCO2(g); log[fCO2(g)]=
pH (-log[aH+]); pmH(-log[mH+]) 5.3205 5.9141 3.400E-02 -1.47
fCO2(g); log[fCO2(g)]=
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: "All-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 titrate 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 <i>not</i> 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 ($< \text{MINABU} \times 1 \times 10^{-6}$)
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 H₂O 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 , $i=1, \dots, N_s$, is added to each beaker. The first volume addition is always zero, that is, $\Delta V_1=0$. 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	$\Delta V_i = DV(2) \times (i-1)$, $i=2, \dots, N_s$, 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	$\Delta V_i = DV(2) \times e^{(i-2)R}$, $i=2, \dots, N_s$, 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	$\Delta V_i = DV(i)$, $i=2, \dots, N_s$, 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

$\Delta V_i = 0.1 \times (i-1)$ mL for 'LINEAR'

$\Delta V_i = 0.1 \times \exp[(i-2)R]$ with $R = (\ln(10.0) - \ln(0.1)) / 13.0$,

$i=2, \dots, 15$ 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 1-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 $i=2, \dots, \text{NSPACE}$.

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.

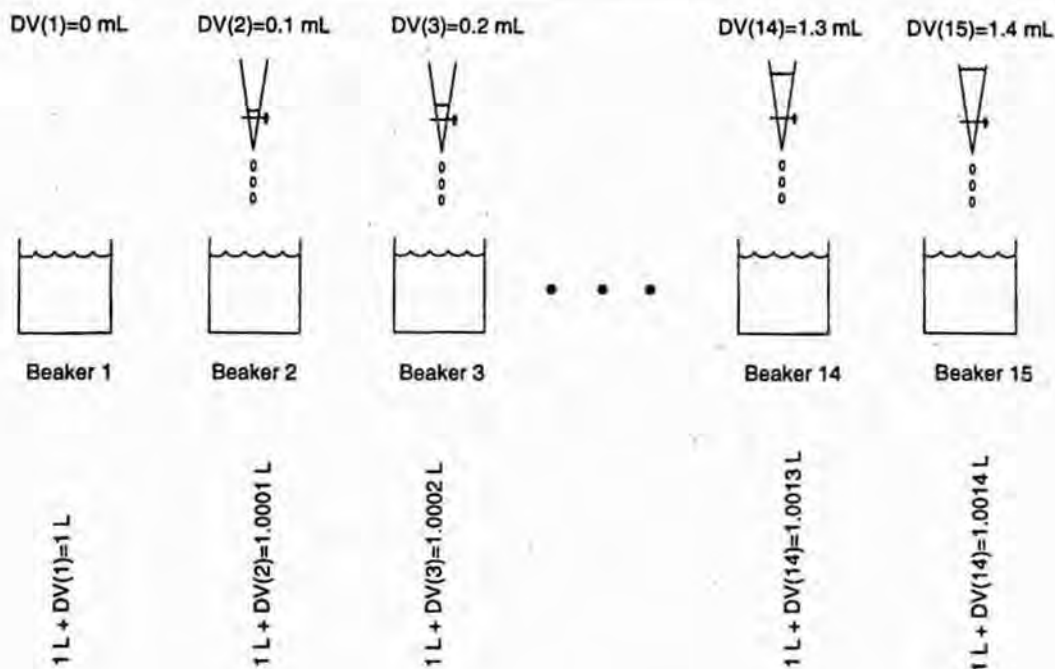


Figure 5. Titration problem using LINEAR option.

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 $\text{Np(V)/CO}_3/\text{NaCl}$ problem illustrates a typical way in which FMT is used. This calculation is designed to show how the solubility of $\text{NaNpO}_2\text{CO}_3(\text{s})$ 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 <i>not</i> 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 <i>not</i> 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

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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 Na₂CO₃·7H₂O(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 NaNpO₂CO₃(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 NaNpO₂CO₃(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 CO₃²⁻ concentration varies widely, from 3.09×10⁻⁸ to 4.84×10⁻² molal (Lines 44-58), as was intended. The NaNpO₂CO₃(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 NpO₂⁺, NpO₂OH(aq), NpO₂(OH)₂⁻, NpO₂CO₃⁻, NpO₂(CO₃)₂³⁻, and NpO₂(CO₃)₃⁵⁻, 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).

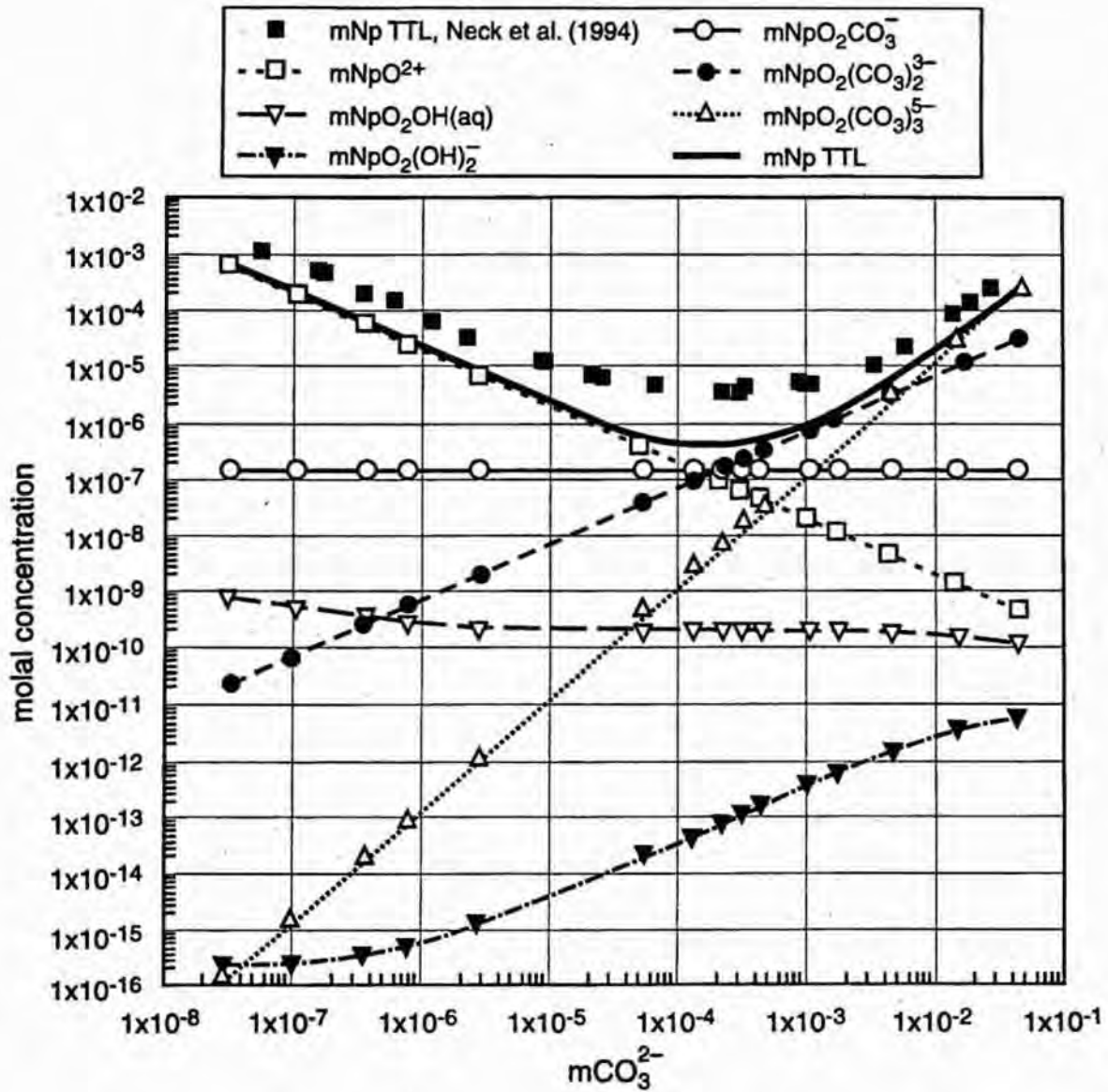
The data from Neck et al. (1994) plotted in Figure 6 are:

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			

INFORMATION ONLY

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 $\text{NpO}_2\text{OH}(\text{aq})$ and $\text{NpO}_2(\text{OH})_2^-$ are unimportant under these conditions, with concentrations always at least three orders of magnitude smaller than the total $\text{Np}(\text{V})$. 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.



TRI-6342-5130-0

Figure 6. Calculated Total Np(V) and Np(V) Concentrations as a function of CO₃²⁻ 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.

INFORMATION ONLY

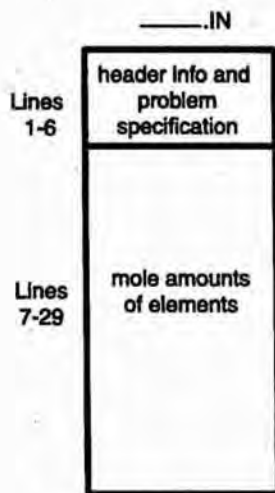
7.1 INPUT

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.



TRI-6342-5131-0

Figure 7. Batch INPUT file.

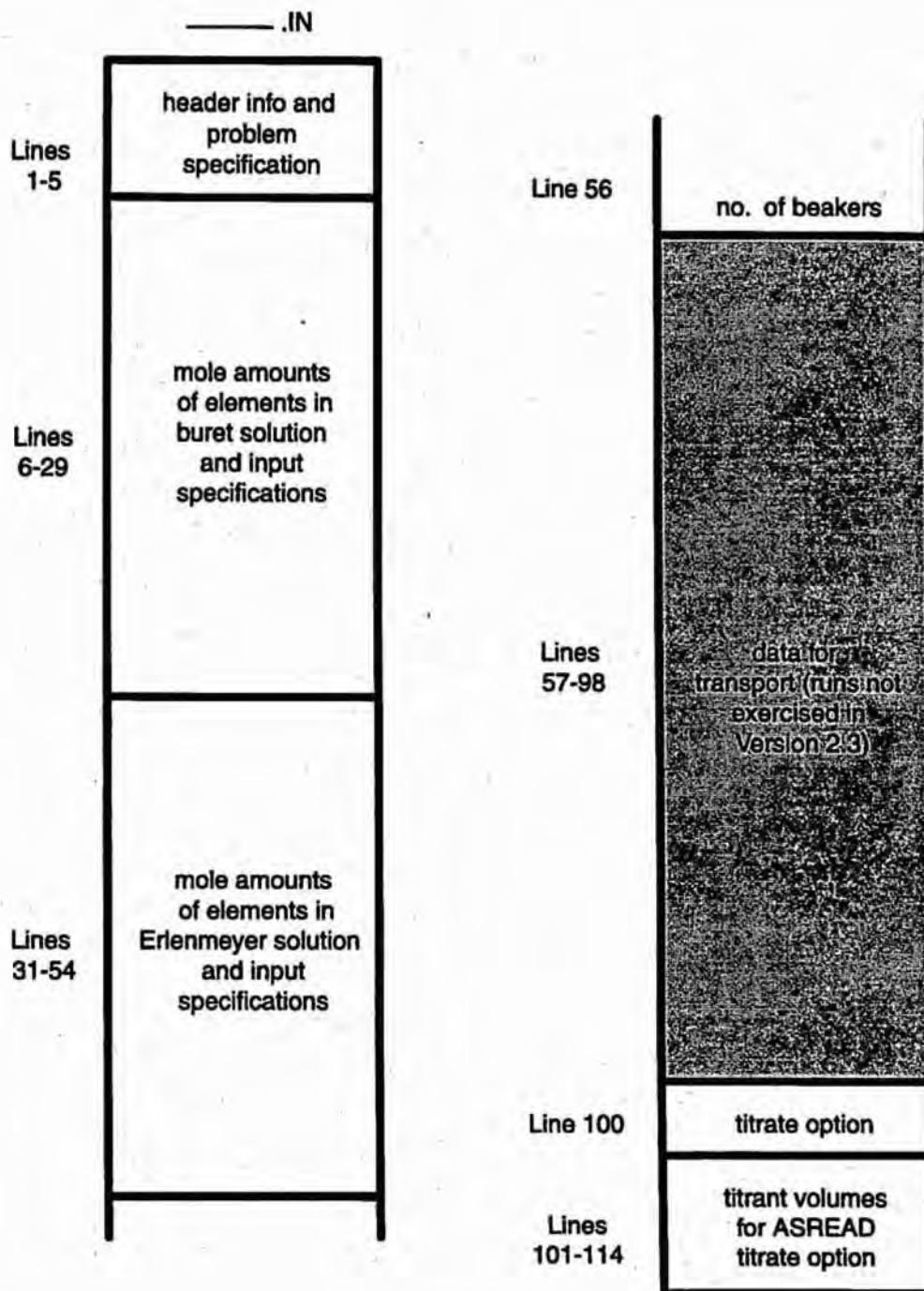
Table 5. INPUT File Parameters for Batch (See Appendix E for sample listing.)

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' or 'nMOLES' 'nEXACT'	two character strings used as flags for calculating the equilibrium state using either: species abundances read from INGUESS from which FMT calculates element abundances 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.



TRI-6342-5132-0

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 Titrant (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	'MOLES' 'EXACT' or 'nMOLES' 'nEXACT'	two character strings used as flags for the titrant or buret solution for calculating the equilibrium state using either: species abundances read from INGUESS from which FMT calculates element abundances 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	'MOLES' 'EXACT' or 'nMOLES' 'nEXACT'	two character strings used as flags for the solution to be titrated or Erlenmeyer solution for calculating the equilibrium state using either: species abundances read from INGUESS from which FMT calculates element abundances 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.
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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 H₂O 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. INGUSS File Parameters for Titrant 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

(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 ₂ O 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

		<p>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 it easy to determine whether errors were made when changing the CHEMDAT file.</p> <p style="text-align: center;">***CAUTION***</p> <p style="text-align: center;">THE USER MUST NOT ALTER THE CHEMDAT FILE WHEN IT IS BEING USED FOR WIPP PA CALCULATIONS.</p>
864	DUMMY, NEQACT	<p>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 ²²Na and ²³Na (which would have to be declared as separate elements in the element list), but instead of repeating all the ²³Na parameters for ²²Na, 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.</p>
866	RPLWCHG	<p>positive integer indicating the element to RePLace With CHArGe. Used to implement the constraint of solution charge neutrality. The 2nd element corresponds to oxygen.</p>
867	DUMMY, NEHRXN	<p>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.</p>

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.
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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

INFORMATION ONLY

	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
	PIZTSI(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: $\sum \text{FORMULA}(j,i) * \text{MWELEM}(j)$, 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,ttelem	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 , ρ_{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.

INFORMATION ONLY

- 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 H₂O 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]

INFORMATION ONLY

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'

INFORMATION ONLY

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 $\text{MINABU} \times 10^{-6}$ (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 equilibrium 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

INFORMATION ONLY

32	PRESSUR, TEMPERA	pressure and temperature for batch problem
34-61	ABUND(i)	table of Elemental Abundances "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 ₂ O, for all species including solids. However, the entry for water is not molality of water, which is invariant, but the mole fraction H ₂ O 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)	pH: 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 $\sum_{i=2}^{N_{\text{spec}}} z_i^2 m_i$, 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 $\text{CO}_2(\text{g})$ (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	$\Sigma\text{CHEMPOT}(i) \times \text{NMOLES}(i)$	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 H₂O 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 Titrant (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 ₂ O)	moles of the i th species normalized to 1 kg H ₂ O (numerically equivalent to molality) $\left[\frac{\text{nmoles}(i)}{\text{nmoles}(\text{H}_2\text{O}) * \text{mwH}_2\text{O}} \right] * 1\text{kg H}_2\text{O}$
	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

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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.

```
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): batch_doc
4 %CMS-I-LIBIS, library is WPSNONPA_CMSROOT:[FMT]
5 %CMS-S-LIBSET, library set
6 -CMS-I-SUPERSEDE, library list superseded
7
8 Elements in CMS Library WPSNONPA_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   WPSNONPA_CMSROOT:[FMT]
17
18 %CMS-S-FETCHED, generation 1 of element WPSNONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched
19
20 Elements in CMS Library WPSNONPA_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   WPSNONPA_CMSROOT:[FMT]
28
29 %CMS-S-FETCHED, generation 1 of element WPSNONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.RHOMIN fetched
30 Enter "Y" or "y" to echo database in OUT file: y
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: "All-14"
37
38 DG_BYPASS flag set to nDG_BYPASS
39 [.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs           FMT V2.3
40 DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-Cl-C1O4 (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 Finished do 10: read b(0) b(1) b(2) cphi
49 Finished do 20: read theta(c,c)
50 Finished do 30: read theta(a,a)
51 Finished do 40: read psi(c,c,a)
52 Finished do 50: read psi(a,a,c)
53 Finished do 55: read neuca(n,c)
54 Finished do 65: read neuani(n,a)
55 Finished do 66: read ptztsi(n,c,a)
56 using PITZER ACTIVITY COEFFICIENT model
57 Charge Balance replaces element Oxygen
58
59 Char Flags: FLOW/BATCH/TITRATE: BATCH      UNUSED
60 this is a BATCH problem
61
62 Echo of Mole Specifications: nMOLES      nEXACT
63 ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH
64 110.2223640000000 Hydrogen
65 55.1654821000000 Oxygen
66 0.200000000000000 Sodium
67 1.000000000000000E-002 Potassium
68 1.000000000000000E-003 Magnesium
69 1.000000000000000E-004 Calcium
70 0.110000000000000 Chlorine
71 1.000000000000000E-003 Sulfur
72 1.000000000000000E-004 Carbon
73 0.000000000000000E+000 PosIon
74 0.000000000000000E+000 NegIon
75 0.000000000000000E+000 Air
76 1.000000000000000E-007 Boron
77 0.000000000000000E+000 Bromine
78 0.000000000000000E+000 TracerEl
79 0.000000000000000E+000 Th(IV)
80 0.000000000000000E+000 Am(III)
81 0.000000000000000E+000 U(VI)
82 0.000000000000000E+000 Np(V)
83 0.000000000000000E+000 ClO4-(EL)
```


INFORMATION ONLY

FMT, Version 2.3
User's Manual, Version 1.1

WPO # 43037
January 9, 1997
Page 104

Appendix A: Sample Screen Display of BATCH_DOC

```
84 0.0000000000000000E+000 Phosphorus
85 0.0000000000000000E+000 Electron
86 4.9060539200000000E-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.

```
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_log
4 *CMS-I-LIBIS, library is WPSNONPA_CMSROOT:[FMT]
5 *CMS-S-LIBSET, library set
6 -CMS-I-SUPERSEDE, library list superseded
7
8 Elements in CMS Library WPSNONPA_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 WPSNONPA_CMSROOT:[FMT]
17
18 *CMS-S-FETCHED, generation 1 of element WPSNONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched
19
20 Elements in CMS Library WPSNONPA_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 WPSNONPA_CMSROOT:[FMT]
28
29 *CMS-S-FETCHED, generation 1 of element WPSNONPA_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: "All-14"
37
38 DG_BYPASS flag set to nDG_BYPASS
39 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
40 DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-Cl-C1O4 (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)}= 5.3205 5.9141 2.171E-07 -6.66
67 pH (-log(aH+)); pmH(-log(mH+)) 5.3205 5.9141 3.400E-02 -1.47
68 fCO2(g); log{fCO2(g)}=
69 TITRATION Character Flags
70 cdum1= TITRATE cdum2= LOG10
71 First Volume Added = 0.10 mL
72 Final Volume Added = 10.00 mL
73
74 pH (-log(aH+)); pmH(-log(mH+)) 5.3205 5.9141 3.400E-02 -1.47
75 fCO2(g); log{fCO2(g)}= 5.6451 6.2386 2.716E-02 -1.57
76 pH (-log(aH+)); pmH(-log(mH+)) 5.9936 6.5870 1.847E-02 -1.73
77 fCO2(g); log{fCO2(g)}= 7.9427 8.5360 3.555E-04 -3.45
78 pH (-log(aH+)); pmH(-log(mH+)) 8.8722 9.4653 4.250E-05 -4.37
79 fCO2(g); log{fCO2(g)}=
80 pH (-log(aH+)); pmH(-log(mH+))
81 fCO2(g); log{fCO2(g)}=
82 pH (-log(aH+)); pmH(-log(mH+))
83 fCO2(g); log{fCO2(g)}=
```

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 WPSNONPA_CMSROOT:[FMT]
5 %CMS-S-LIBSET, library set
6 -CMS-I-SUPERSEDE, library list superseded
7
8 Elements in CMS Library WPSNONPA_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   WPSNONPA_CMSROOT:[FMT]
17
18 %CMS-S-FETCHED, generation 1 of element WPSNONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTEST.CHEMDAT fetched
19
20 Elements in CMS Library WPSNONPA_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   WPSNONPA_CMSROOT:[FMT]
28
29 %CMS-S-FETCHED, generation 1 of element WPSNONPA_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: *All-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 neuca(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+]); pM(-log[mH+])    11.7497      11.6199
66 fCO2(g); log[fCO2(g)]=          2.171E-07    -6.66
67 pH (-log[aH+]); pM(-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 WPSNONPA_CMSROOT:[FMT]
5 %CMS-S-LIBSET, library set
6 -CMS-I-SUPERSEDE, library list superseded
7
8 Elements in CMS Library WPSNONPA_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_RTTEST.CHEMDAT "CHEMDAT DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING"
14 Select CHEMDAT name from list above: FMT_HMW_NP_AM_RTTEST.CHEMDAT
15 Your CMS library list consists of:
16   WPSNONPA_CMSROOT:[FMT]
17
18 %CMS-S-FETCHED, generation 1 of element WPSNONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTTEST.CHEMDAT fetched
19
20 Elements in CMS Library WPSNONPA_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_RTTEST.RHOMIN "RHOMIN DATA BASE FILE FOR FMT 2.3 REGRESSION TESTING"
25 Select RHOMIN name from list above: FMT_HMW_NP_AM_RTTEST.RHOMIN
26 Your CMS library list consists of:
27   WPSNONPA_CMSROOT:[FMT]
28
29 %CMS-S-FETCHED, generation 1 of element WPSNONPA_CMSROOT:[FMT]FMT_HMW_NP_AM_RTTEST.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: "All-14"
37
38 DG_BYPASS flag set to nDG_BYPASS
39 Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl
40 DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-Cl-C1O4 (NR94);
41 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,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[mH+]); pmH(-log[mH+])    11.7497      11.6199
66 fCO2(g); log{fCO2(g)}=           2.171E-07    -6.66
67 pH (-log[mH+]); 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
```

FMT V2.3

Appendix D Sample Screen Display of Np_NaCl_BM

72	First Volume Added =	0.10 mL			
73	Final Volume Added =	10.00 mL			
74					
75	pH (-log[aH+]); pmH(-log[mH+])	5.3205	5.9141		
76	fCO2(g); log[fCO2(g)] =			3.400E-02	-1.47
77	pH (-log[aH+]); pmH(-log[mH+])	5.6451	6.2386		
78	fCO2(g); log[fCO2(g)] =			2.716E-02	-1.57
79	pH (-log[aH+]); pmH(-log[mH+])	5.9936	6.5870		
80	fCO2(g); log[fCO2(g)] =			1.847E-02	-1.73
81	pH (-log[aH+]); pmH(-log[mH+])	6.2353	6.8286		
82	fCO2(g); log[fCO2(g)] =			1.290E-02	-1.89
83	pH (-log[aH+]); pmH(-log[mH+])	6.6996	7.2930		
84	fCO2(g); log[fCO2(g)] =			5.484E-03	-2.26
85	pH (-log[aH+]); pmH(-log[mH+])	7.9427	8.5359		
86	fCO2(g); log[fCO2(g)] =			3.555E-04	-3.45
87	pH (-log[aH+]); pmH(-log[mH+])	8.3317	8.9250		
88	fCO2(g); log[fCO2(g)] =			1.461E-04	-3.84
89	pH (-log[aH+]); pmH(-log[mH+])	8.5655	9.1587		
90	fCO2(g); log[fCO2(g)] =			8.559E-05	-4.07
91	pH (-log[aH+]); pmH(-log[mH+])	8.7166	9.3098		
92	fCO2(g); log[fCO2(g)] =			6.060E-05	-4.22
93	pH (-log[aH+]); pmH(-log[mH+])	8.8722	9.4653		
94	fCO2(g); log[fCO2(g)] =			4.250E-05	-4.37
95	pH (-log[aH+]); pmH(-log[mH+])	9.2225	9.8154		
96	fCO2(g); log[fCO2(g)] =			1.922E-05	-4.72
97	pH (-log[aH+]); pmH(-log[mH+])	9.4695	10.0620		
98	fCO2(g); log[fCO2(g)] =			1.108E-05	-4.96
99	pH (-log[aH+]); pmH(-log[mH+])	9.8493	10.4406		
100	fCO2(g); log[fCO2(g)] =			4.873E-06	-5.31
101	pH (-log[aH+]); pmH(-log[mH+])	10.2955	10.8825		
102	fCO2(g); log[fCO2(g)] =			2.019E-06	-5.69
103	pH (-log[aH+]); pmH(-log[mH+])	10.6594	11.2341		
104	fCO2(g); log[fCO2(g)] =			1.106E-06	-5.96
105	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.

```
1 'Benchmark TITRATE Problem, LOG10 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)  
49 0.00000000E+00 U(VI)  
50 1.00000000E+01 Np(V)  
51 0.00000000E+00 ClO4-(EL)  
52 0.00000000E+00 Phosphorus  
53 0.00000000E+00 Electron  
54 -2.37316632E-15 Charge  
55  
56 15 2.25d3 0.0025d0 1.80001d5 'nDXVARIABLE'  
57 'nDIFFUS',  
58 'CONVEC',
```

Appendix F: Sample Input File "Np_NaCl_BM_LOG.IN"

```
59 'nSSDIFF',
60 'nRESTART',
61 'nPUSHPULL', 'nMULTINJ',
62
63 20 1 20 'nLOTS' 10
64 'nTGRAD' 'LINEAR'
65 'FRAC FLO' 'nTWO PHASE' 'nMASS TR'
66 3
67 0.1d0 0.2d0 0.3d0
68 1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'
69 'nMOLES' 'nEXACT' Plain old pure H2O
70 1.11017364E+02 Hydrogen
71 5.55086820E+01 Oxygen
72 0.00000000E+00 Sodium
73 0.00000000E+00 Potassium
74 0.00000000E+00 Magnesium
75 0.00000000E+00 Calcium
76 0.00000000E+00 Chlorine
77 0.00000000E+00 Sulfur
78 0.00000000E+00 Carbon
79 0.00000000E+00 PosIon
80 0.00000000E+00 NegIon
81 0.00000000E+00 Air
82 0.00000000E+00 Boron
83 0.00000000E+00 Bromine
84 0.00000000E+00 TracerEl
85 0.00000000E+00 Pu(III)
86 0.00000000E+00 Am(III)
87 0.00000000E+00 U(VI)
88 0.00000000E+00 Np(V)
89 0.00000000E+00 ClO4- (EL)
90 0.00000000E+00 Phosphorus
91 0.00000000E+00 Electron
92 0.00000000E+00 Charge
93
94 1.d-12 1.d-20 (fracture, matrix permeabilities)
95 'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)
96 'VAR_AQ_RHO' 1074.9d0
97 'nNO X DIFF',
98 'UNIFORM', 0
99
100 '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 E (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"

```
49 0.00000000E+00 U(VI)
50 1.00000000E+01 Np(V)
51 0.00000000E+00 ClO4-(EL)
52 0.00000000E+00 Phosphorus
53 0.00000000E+00 Electron
54 -2.37316632E-15 Charge
55
56 15 2.25d3 0.0025d0 1.800001d5 'NDXVARIABLE'
57 'nDIFFUS',
58 'CONVEC',
59 'nSSDIFF',
60 'nRESTART',
61 'nPUSHPULL', 'nMULTINJ',
62
63 20 1 20 'nLOTS' 10
64 'nTGRAD' 'LINEAR'
65 'FRAC FLO' 'nTWO PHASE' 'nMASS TR'
66 3
67 0.1d0 0.2d0 0.3d0
68 1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'
69 'nMOLES' 'nEXACT' Plain old pure H2O
70 1.11017364E+02 Hydrogen
71 5.55086820E+01 Oxygen
72 0.00000000E+00 Sodium
73 0.00000000E+00 Potassium
74 0.00000000E+00 Magnesium
75 0.00000000E+00 Calcium
76 0.00000000E+00 Chlorine
77 0.00000000E+00 Sulfur
78 0.00000000E+00 Carbon
79 0.00000000E+00 PosIon
80 0.00000000E+00 NegIon
81 0.00000000E+00 Air
82 0.00000000E+00 Boron
83 0.00000000E+00 Bromine
84 0.00000000E+00 TracerEl
85 0.00000000E+00 Pu(III)
86 0.00000000E+00 Am(III)
87 0.00000000E+00 U(VI)
88 0.00000000E+00 Np(V)
89 0.00000000E+00 ClO4-(EL)
90 0.00000000E+00 Phosphorus
91 0.00000000E+00 Electron
92 0.00000000E+00 Charge
93
94 1.d-12 1.d-20 (fracture, matrix permeabilities)
95 'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)
96 'VAR_AQ_RHO' 1074.9d0
97 'nNO X DIFF',
98 'UNIFORM', 0
99
100 '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"

```
49 0.00000000E+00 U(VI)
50 1.00000000E+01 Np(V)
51 0.00000000E+00 ClO4-(EL)
52 0.00000000E+00 Phosphorus
53 0.00000000E+00 Electron
54 -2.37316632E-15 Charge
55
56 15 2.25d3 0.0025d0 1.800001d5 'NDXVARIABLE'
57 'NDIFFUS',
58 'CONVEC',
59 'NSSDIFF',
60 'nRESTART',
61 'nPUSHPULL', 'nMULTINJ',
62
63 20 1 20 'nLOTS' 10
64 'nTGRAD' 'LINEAR'
65 'FRAC FLO' 'nTWO PHASE' 'nMASS TR'
66 3
67 0.1d0 0.2d0 0.3d0
68 1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIP' 'LHSFDIP'
69 'nMOLES' 'nEXACT' Plain old pure H2O
70 1.11017364E+02 Hydrogen
71 5.55086820E+01 Oxygen
72 0.00000000E+00 Sodium
73 0.00000000E+00 Potassium
74 0.00000000E+00 Magnesium
75 0.00000000E+00 Calcium
76 0.00000000E+00 Chlorine
77 0.00000000E+00 Sulfur
78 0.00000000E+00 Carbon
79 0.00000000E+00 PosIon
80 0.00000000E+00 NegIon
81 0.00000000E+00 Air
82 0.00000000E+00 Boron
83 0.00000000E+00 Bromine
84 0.00000000E+00 TracerEl
85 0.00000000E+00 Pu(III)
86 0.00000000E+00 Am(III)
87 0.00000000E+00 U(VI)
88 0.00000000E+00 Np(V)
89 0.00000000E+00 ClO4-(EL)
90 0.00000000E+00 Phosphorus
91 0.00000000E+00 Electron
92 0.00000000E+00 Charge
93
94 1.d-12 1.d-20 (fracture, matrix permeabilities)
95 'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)
96 'VAR_AQ_RHO' 1074.9d0
97 'nNO X DIFF',
98 'UNIFORM', 0
99
100 'TITRATE', 'ASREAD', 0.1d0, 10.d0, 'nINJSOLIDS'
101 0.10000
102 0.14251
103 0.16
104 0.18
105 0.20309
106 0.22
107 0.24
108 0.26
109 0.28943
110 0.41246
111 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

230	3	.0	.0	.0	.0	Hg++ PO4--		
231								
232	1	-.10	1.658	.0	.0	HgOH+ Cl-	10W84	
233	1	.0	.0	.0	.0	HgOH+ SO4-	10W84	
234	1	.0	.0	.0	.0	HgOH+ HSO4-	10W84	
235	1	.0	.0	.0	.0	HgOH+ OH-	10W84	
236	1	.0	.0	.0	.0	HgOH+ HCO3-	10W84	
237	1	.0	.0	.0	.0	HgOH+ CO3-	10W84	
238	1	.0	.0	.0	.0	HgOH+ B(OH)4-		
239	1	.0	.0	.0	.0	HgOH+ B(OH)4-		
240	1	.0	.0	.0	.0	HgOH+ B(OH)4-		
241	1	.0	.0	.0	.0	HgOH+ Br-		
242	1	.0	.0	.0	.0	HgOH+ Am(CO3)2-		
243	1	.0	.0	.0	.0	HgOH+ Am(CO3)3--		
244	1	.0	.0	.0	.0	HgOH+ ClO4-		
245	1	.0	.0	.0	.0	HgOH+ HPO2(OH)2-		
246	1	.0	.0	.0	.0	HgOH+ HPO2CO3-		
247	1	.0	.0	.0	.0	HgOH+ HPO2(CO3)2--		
248	1	.0	.0	.0	.0	HgOH+ HPO2(CO3)3---		
249	1	.0	.0	.0	.0	HgOH+ H2PO4-		
250	1	.0	.0	.0	.0	HgOH+ HPO4-		
251	1	.0	.0	.0	.0	HgOH+ PO4--		
252								
253	1	.1775	.2945	.0	.0008	H+ Cl-	10W84	
254	1	.0298	.0	.0	.0438	H+ SO4-	10W84	
255	1	.2065	.5556	.0	.0	H+ HSO4-	10W84	
256	1	.0	.0	.0	.0	H+ OH-	10W84	
257	1	.0	.0	.0	.0	H+ HCO3-	10W84	
258	1	.0	.0	.0	.0	H+ CO3-	10W84	
259	1	.0	.0	.0	.0	H+ B(OH)4-	FW86	
260	1	.0	.0	.0	.0	H+ B(OH)4-	FW86	
261	1	.0	.0	.0	.0	H+ B(OH)4-	FW86	
262	1	.0	.0	.0	.0	H+ Br-	FW86	
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+ HPO2(OH)2-		
267	1	.0	.0	.0	.0	H+ HPO2CO3-		
268	1	.0	.0	.0	.0	H+ HPO2(CO3)2--		
269	1	.0	.0	.0	.0	H+ HPO2(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	HgB(OH)4+ Cl-	10W84	
275	1	.0	.0	.0	.0	HgB(OH)4+ SO4-	10W84	
276	1	.0	.0	.0	.0	HgB(OH)4+ HSO4-	10W84	
277	1	.0	.0	.0	.0	HgB(OH)4+ OH-	10W84	
278	1	.0	.0	.0	.0	HgB(OH)4+ HCO3-	10W84	
279	1	.0	.0	.0	.0	HgB(OH)4+ CO3-	10W84	
280	1	.0	.0	.0	.0	HgB(OH)4+ B(OH)4-		
281	1	.0	.0	.0	.0	HgB(OH)4+ B(OH)4-		
282	1	.0	.0	.0	.0	HgB(OH)4+ B(OH)4-		
283	1	.0	.0	.0	.0	HgB(OH)4+ B(OH)4-		
284	1	.0	.0	.0	.0	HgB(OH)4+ Br-		
285	1	.0	.0	.0	.0	HgB(OH)4+ Am(CO3)2-		
286	1	.0	.0	.0	.0	HgB(OH)4+ Am(CO3)3--		
287	1	.0	.0	.0	.0	HgB(OH)4+ ClO4-		
288	1	.0	.0	.0	.0	HgB(OH)4+ HPO2(OH)2-		
289	1	.0	.0	.0	.0	HgB(OH)4+ HPO2CO3-		
290	1	.0	.0	.0	.0	HgB(OH)4+ HPO2(CO3)2--		
291	1	.0	.0	.0	.0	HgB(OH)4+ HPO2(CO3)3---		
292	1	.0	.0	.0	.0	HgB(OH)4+ H2PO4-		
293	1	.0	.0	.0	.0	HgB(OH)4+ HPO4-		
294	1	.0	.0	.0	.0	HgB(OH)4+ PO4--		
295	1	.12	.0	.0	.0	CaB(OH)4+ Cl-	10W84	
296	1	.0	.0	.0	.0	CaB(OH)4+ SO4-	10W84	
297	1	.0	.0	.0	.0	CaB(OH)4+ HSO4-	10W84	
298	1	.0	.0	.0	.0	CaB(OH)4+ OH-	10W84	
299	1	.0	.0	.0	.0	CaB(OH)4+ HCO3-	10W84	
300	1	.0	.0	.0	.0	CaB(OH)4+ CO3-	10W84	
301	1	.0	.0	.0	.0	CaB(OH)4+ B(OH)4-		
302	1	.0	.0	.0	.0	CaB(OH)4+ B(OH)4-		
303	1	.0	.0	.0	.0	CaB(OH)4+ B(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+ HPO2(OH)2-		
309	1	.0	.0	.0	.0	CaB(OH)4+ HPO2CO3-		
310	1	.0	.0	.0	.0	CaB(OH)4+ HPO2(CO3)2--		
311	1	.0	.0	.0	.0	CaB(OH)4+ HPO2(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	-.0284	Am+++ Cl-	FRS89	
317	1	.0398	.0	-.2500	.0	Am+++ SO4-	RFP94	
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	1	.0	.0	.0	.0	Am+++ CO3-		
322	1	.0	.0	.0	.0	Am+++ B(OH)4-		
323	1	.0	.0	.0	.0	Am+++ B(OH)4-		
324	1	.0	.0	.0	.0	Am+++ B(OH)4-		
325	1	.0	.0	.0	.0	Am+++ Br-		
326	1	.0	.0	.0	.0	Am+++ Am(CO3)2-		
327	1	.0	.0	.0	.0	Am+++ Am(CO3)3--		
328	1	.80	5.35	.0	-.0048	Am+++ ClO4-	FRF90	
329	1	.0	.0	.0	.0	Am+++ HPO2(OH)2-		
330	1	.0	.0	.0	.0	Am+++ HPO2CO3-		
331	1	.0	.0	.0	.0	Am+++ HPO2(CO3)2--		
332	1	.0	.0	.0	.0	Am+++ HPO2(CO3)3---		
333	1	.0	.0	.0	.0	Am+++ H2PO4-	RFP94	
334	1	.0	.0	.0	.0	Am+++ HPO4-		
335	1	.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+ B(OH)4-		
345	1	.0	.0	.0	.0	AmCO3+ B(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+ HPO2(OH)2-		
351	1	.0	.0	.0	.0	AmCO3+ HPO2CO3-		
352	1	.0	.0	.0	.0	AmCO3+ HPO2(CO3)2--		
353	1	.0	.0	.0	.0	AmCO3+ HPO2(CO3)3---		

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

Rai, D., A.R. Felmy, and R.W. Fulton. 1992a. "Solubility and Ion Activity Product of $\text{AmPO}_4 \cdot x\text{H}_2\text{O}(\text{am})$." *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 $\text{NdPO}_4(\text{c})$ 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 R.W. Fulton. 1994. "Solubility of $\text{NaNd}(\text{CO}_3)_2 \cdot 6\text{H}_2\text{O}$ 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.

```

1 CHEMDAT file name is U1:\GC8ABB.PVT\HM\HMW_NP_AM_RTEST.CHEMDAT;
2 Temperature is Hard Coded as 298.15K
3 (.PD.TITRATE\BATCH.DOC.IN; to illustrate/document "BATCH" runs
4 DATABASE: H0984/PW86; H0(V)-Na-CO3-OH-C1O4 (H094);
5 95.01.31 Am(III)-Na-C1-CO3-SO4-PO4 (P0989,P0990,P91,R0992,R0994)
6
7 Accuracy of reactions is 1.0000E-06
8 Minimum elemental abundance is 1.0000E-18
9 Number of Aqueous Species is 50
10
11 Species Order for Pitzer Parameters
12
13 Cations 13
14
15 Na+
16 Mg(OH)4+
17 K+
18 Ca(OH)4+
19 Ca++
20 Am+++
21 Mg++
22 AmCO3+
23 MgOH+
24 Th+++
25 H+
26 UO2++
27
28 Anions 20
29
30 Cl-
31 B(OH)4-
32 ClO4-
33 HPO4-
34 SO4-
35 B(OH)4-
36 B(OH)2-
37 PO4-
38 HSO4-
39 B(OH)4-
40 B(OH)2-
41 H2PO4-
42 OH-
43 Br-
44 HPO2(CO3)2-
45 HCO3-
46 Am(CO3)2-
47 HPO2(CO3)3-
48 CO3-
49 HCO3-
50 Am(CO3)3-
51 H2PO4-
52
53 Neutral 6
54
55 CO2(aq)
56 CaCO3(aq)
57 MgCO3(aq)
58 B(OH)2(aq)
59 HPO2OH(aq)
60 H3PO4(aq)
61
62 Cation-Anion Binary Interaction Parameters
63
64 Cation Anion Beta(0) Beta(1) Beta(2) Cphi Alpha-Values
65
66 Na+ Cl- 0.07650 0.26440 0.00000 0.00137 (2.0,12) 1-1,1-2,1-3
67 Na+ SO4- 0.01958 1.11300 0.00000 0.00497 (2.0,12) 1-1,1-2,1-3
68 Na+ HSO4- 0.04540 0.39800 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
69 Na+ OH- 0.08640 0.25300 0.00000 0.00440 (2.0,12) 1-1,1-2,1-3
70 Na+ HCO3- 0.02770 0.04110 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
71 Na+ CO3- 0.03990 0.28900 0.00000 0.01140 (2.0,12) 1-1,1-2,1-3
72 Na+ B(OH)4- -0.04270 0.08900 0.00000 0.00440 (2.0,12) 1-1,1-2,1-3
73 Na+ B(OH)2- -0.05600 -0.91000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
74 Na+ B(OH)2- -0.11000 -0.40000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
75 Na+ Br- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
76 Na+ Am(CO3)2- 0.00000 -8.37000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
77 Na+ Am(CO3)3- -0.94000 8.10000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
78 Na+ ClO4- 0.05540 0.27550 0.00000 0.41800 (2.0,12) 1-1,1-2,1-3
79 Na+ HPO2(OH)2- 0.00000 0.00000 0.00000 -0.00118 (2.0,12) 1-1,1-2,1-3
80 Na+ HPO2CO3- 0.16100 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
81 Na+ HPO2(CO3)2- 0.40700 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
82 Na+ HPO2(CO3)3- 1.97000 16.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
83 Na+ H2PO4- -0.05330 0.03960 0.00000 0.02940 (2.0,12) 1-1,1-2,1-3
84 Na+ HPO4- -0.05830 1.46600 0.00000 0.00795 (2.0,12) 1-1,1-2,1-3
85 Na+ PO4- 0.17810 3.85100 0.00000 -0.05154 (2.0,12) 1-1,1-2,1-3
86
87 K+ Cl- 0.04835 0.21220 0.00000 -0.00084 (2.0,12) 1-1,1-2,1-3
88 K+ SO4- 0.04995 0.77930 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
89 K+ HSO4- -0.00010 0.17350 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
90 K+ OH- 0.12980 0.32000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
91 K+ HCO3- 0.02960 -0.01300 0.00000 -0.00800 (2.0,12) 1-1,1-2,1-3
92 K+ CO3- 0.14880 1.43000 0.00000 -0.00150 (2.0,12) 1-1,1-2,1-3
93 K+ B(OH)4- 0.03500 0.14000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
94 K+ B(OH)2- -0.13000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
95 K+ B(OH)2- -0.02000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
96 K+ Br- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
97 K+ Am(CO3)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
98 K+ Am(CO3)3- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
99 K+ ClO4- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
100 K+ HPO2(OH)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
101 K+ HPO2CO3- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
102 K+ HPO2(CO3)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
103 K+ HPO2(CO3)3- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
104 K+ H2PO4- -0.06780 -0.10420 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
105 K+ HPO4- 0.02480 1.27400 0.00000 0.01640 (2.0,12) 1-1,1-2,1-3
106 K+ PO4- 0.37290 3.97200 0.00000 -0.08680 (2.0,12) 1-1,1-2,1-3
107
108 Ca++ Cl- 0.31590 1.61400 0.00000 -0.00034 (2.0,12) 1-1,1-2,1-3
109 Ca++ SO4- 0.20000 3.19730 0.00000 0.00000 (1.4,12) 2-2
110 Ca++ HSO4- 0.21450 2.53000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
111 Ca++ OH- -0.17470 -0.23030 -5.72000 0.00000 (2.0,12) 1-1,1-2,1-3
112 Ca++ HCO3- 0.40000 2.97700 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
113 Ca++ CO3- 0.00000 0.00000 0.00000 0.00000 (1.4,12) 2-2
114 Ca++ B(OH)4- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
115 Ca++ B(OH)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
116 Ca++ B(OH)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
117 Ca++ Br- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
118 Ca++ Am(CO3)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
119 Ca++ Am(CO3)3- 0.00000 0.00000 0.00000 0.00000 (1.4,50) 2-(m=2)
120 Ca++ ClO4- 0.45110 1.75600 0.00000 -0.00500 (2.0,12) 1-1,1-2,1-3
121 Ca++ HPO2(OH)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
122 Ca++ HPO2CO3- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
123 Ca++ HPO2(CO3)2- 0.00000 0.00000 0.00000 0.00000 (1.4,50) 2-(m=2)
124 Ca++ HPO2(CO3)3- 0.00000 0.00000 0.00000 0.00000 (1.4,50) 2-(m=2)
125 Ca++ H2PO4- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
126 Ca++ HPO4- 0.00000 0.00000 0.00000 0.00000 (1.4,12) 2-2
127 Ca++ PO4- 0.00000 0.00000 0.00000 0.00000 (1.4,50) 2-(m=2)
128
129 Mg++ Cl- 0.35235 1.68150 0.00000 0.00519 (2.0,12) 1-1,1-2,1-3
130 Mg++ SO4- 0.22100 3.34300 0.00000 0.02500 (1.4,12) 2-2
131 Mg++ HSO4- 0.47460 1.73900 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
132 Mg++ OH- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
133 Mg++ HCO3- 0.32900 0.60720 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
134 Mg++ CO3- 0.00000 0.00000 0.00000 0.00000 (1.4,12) 2-2
135 Mg++ B(OH)4- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
136 Mg++ B(OH)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
137 Mg++ B(OH)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
138 Mg++ Br- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
139 Mg++ Am(CO3)2- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
140 Mg++ Am(CO3)3- 0.00000 0.00000 0.00000 0.00000 (1.4,50) 2-(m=2)
141 Mg++ ClO4- 0.49610 2.04800 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
142 Mg++ HPO2(OH)2- 0.00000 0.00000 0.00000 0.00958 (2.0,12) 1-1,1-2,1-3
143 Mg++ HPO2CO3- 0.00000 0.00000 0.00000 0.00000 (2.0,12) 1-1,1-2,1-3
144

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INFORMATION ONLY

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTST.CHEM.DAT

Line	Label	Value 1	Value 2	Value 3	Value 4	Value 5	Value 6
115	Mg**	Np02 (CO3) 2--	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n+2)
116	Mg**	Np02 (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+	H2O4-	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+	B(O3)(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	0.00000	(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+	H2O4-	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+	B(O3)(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-	0.21710	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
155	H+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00813	(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+	H2O4-	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+	B(O3)(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+	H2O4-	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+	B(O3)(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	5.40300	0.00000	-0.02840	(2.0,12) 1-1,1-2,1-3
206	Am***	SO4-	1.03980	0.00000	-2500.00000	0.00000	(1.4,50) 2-(n+2)
207	Am***	H2O4-	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***	B(O3)(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	-0.09480	(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	(2.0,12) 1-1,1-2,1-3
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+	H2O4-	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+	B(O3)(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		

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-(m=2)		
249	Th++++	H2O4-	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-(m=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-(m=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	(2.0,12)	1-1,1-2,1-3		
263	Th++++	NpO2 (CO3) 3---	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(m=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-(m=2)		
266	Th++++	PO4--	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(m=2)		
267										
268	UO2++	Cl-	0.42740	1.44400	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++	H2O4-	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-(m=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-(m=2)		
284	UO2++	NpO2 (CO3) 3---	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(m=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-(m=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+	H2O4-	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		

Cation-Cation Ternary Interactions: theta(c1,c2)

310											
311											
312											
313	Na+	K+	Ca++	Mg++	MgOH+	H+	MgB (OH) 4+	CaB (OH) 4+	Am+++	AmCO3+	Th++++
314			0.01200	0.07000	0.07000	0.00000	0.03600	0.00000	0.00000	0.00000	0.00000
315	Na+		UO2++	NpO2+							
316			0.00000	0.00000							
317											
318	K+	Ca++	Mg++	MgOH+	H+	MgB (OH) 4+	CaB (OH) 4+	Am+++	AmCO3+	Th++++	UO2++
319			0.03200	0.00000	0.00000	0.00500	0.00000	0.00000	0.00000	0.00000	0.00000
320	K+		NpO2+								
321			0.00000								
322											
323	Ca++	Mg++	MgOH+	H+	MgB (OH) 4+	CaB (OH) 4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+
324			0.00700	0.00000	0.09200	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
325											
326	Mg++	MgOH+	H+	MgB (OH) 4+	CaB (OH) 4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+	
327			0.00000	0.10000	0.00000	0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
328											
329	MgOH+	H+	MgB (OH) 4+	CaB (OH) 4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+		
330			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
331											
332	H+	MgB (OH) 4+	CaB (OH) 4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+			
333			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
334											
335	MgB (OH) 4+	CaB (OH) 4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+				
336			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000			
337											
338	CaB (OH) 4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+					
339			0.00000	0.00000	0.00000	0.00000					
340											
341	Am+++	AmCO3+	Th++++	UO2++	NpO2+						
342			0.00000	0.00000	0.00000						
343											
344	AmCO3+	Th++++	UO2++	NpO2+							
345			0.00000	0.00000	0.00000						
346											
347	Th++++	UO2++	NpO2+								
348			0.00000	0.00000							
349											
350	UO2++	NpO2+									
351			0.00000								

Anion-Anion Ternary Interactions: theta(a1,a2)

352											
353											
354											
355	Cl-	SO4-	H2O4-	OH-	HCO3-	CO3-	B (OH) 4-	B3O3 (OH) 4-	B4O5 (OH) 4-	Br-	Am (CO3) 2-
356		0.02000	-0.00600	-0.05000	0.03600	-0.02000	-0.06500	0.12000	0.07400	0.00000	0.00000
357	Cl-	Am (CO3) 3--	ClO4-	NpO2 (OH) 2-	NpO2CO3-	NpO2 (CO3) 2--	NpO2 (CO3) 3---	H2PO4-	HPO4-	PO4--	
358		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10000	0.00000	0.00000	
359											
360											
361	SO4-	H2O4-	OH-	HCO3-	CO3-	B (OH) 4-	B3O3 (OH) 4-	B4O5 (OH) 4-	Br-	Am (CO3) 2-</	

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTEST.CHEMDAT

859	HC03-	B(OH)4-	0.00000	0.00000	0.00000								
860	HC03-	B3O3(OH)4-	0.00000	0.00000	0.00000								
861	HC03-	B4O5(OH)4-	0.00000	0.00000	0.00000								
862	HC03-	Br-	0.00000	0.00000	0.00000								
863	HC03-	Am(CO3)2-	0.00000	0.00000	0.00000								
864	HC03-	Am(CO3)3--	0.00000	0.00000	0.00000								
865	HC03-	ClO4-	0.00000	0.00000	0.00000								
866	HC03-	NpO2(OH)2-	0.00000	0.00000	0.00000								
867	HC03-	NpO2CO3-	0.00000	0.00000	0.00000								
868	HC03-	NpO2(CO3)2--	0.00000	0.00000	0.00000								
869	HC03-	NpO2(CO3)3---	0.00000	0.00000	0.00000								
870	HC03-	H2PO4-	0.00000	0.00000	0.00000								
871	HC03-	HPO4-	0.00000	0.00000	0.00000								
872	HC03-	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---	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---	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---	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---	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---	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---	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---	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---	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---	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---	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---	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---	H2PO4-	0.00000	0.00000	0.00000								
973	NpO2(CO3)3---	HPO4-	0.00000	0.00000	0.00000								
974	NpO2(CO3)3---	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													
982	Na+	CO3(aq)	0.10000	CaCO3(aq)	0.00000	MgCO3(aq)	0.00000	B(OH)3(aq)	-0.09700	NpO2OH(aq)	0.00000	H3PO4(aq)	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								
1000	Cl-	CO2(aq)	CaCO3(aq)	MgCO3(aq)	B(OH)3(aq)	NpO2OH(aq)	H2PO4(aq)	
1001	SO4=	-0.00500	0.00000	0.00000	0.09100	0.00000	0.00000	
1002	HSO4-	-0.09700	0.00000	0.00000	0.01800	0.00000	0.00000	
1003	OH-	-0.00300	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								
1025	Na+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	
1026	Na+	SO4=	0.00000	0.00000	0.00000	0.04600	0.00000	
1027	Na+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1028	Na+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	
1029	Na+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	
1030	Na+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1031	Na+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1032	Na+	B4O5(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1033	Na+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	
1034	Na+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	
1035	Na+	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	
1036	Na+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1037	Na+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	
1038	Na+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	
1039	Na+	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	
1040	Na+	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	
1041	Na+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1042	Na+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1043	Na+	PO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1044	Na+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	
1045	K+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1046	K+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1047	K+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	
1048	K+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	
1049	K+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	
1050	K+	CO3=	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	
1052	K+	B3O3(OH)4-	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	
1054	K+	Br-	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	
1056	K+	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	
1057	K+	ClO4-	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	
1059	K+	NpO2CO3-	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	
1061	K+	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	
1062	K+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1063	K+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1064	K+	PO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1065	Ca++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	
1066	Ca++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1067	Ca++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1068	Ca++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	
1069	Ca++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	
1070	Ca++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1071	Ca++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1072	Ca++	B4O5(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1073	Ca++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	
1074	Ca++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	
1075	Ca++	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	
1076	Ca++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1077	Ca++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	
1078	Ca++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	
1079	Ca++	NpO2(CO3)2--	0.00000	0.00000	0.00000	0.00000	0.00000	
1080	Ca++	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	
1081	Ca++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1082	Ca++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1083	Ca++	PO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1084	Mg++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	
1085	Mg++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1086	Mg++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1087	Mg++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	
1088	Mg++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	
1089	Mg++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	
1090	Mg++	CO3=	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	
1092	Mg++	B3O3(OH)4-	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	
1094	Mg++	Br-	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	
1096	Mg++	Am(CO3)3--	0.00000	0.00000	0.00000	0.00000	0.00000	
1097	Mg++	ClO4-	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	
1099	Mg++	NpO2CO3-	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	
1101	Mg++	NpO2(CO3)3---	0.00000	0.00000	0.00000	0.00000	0.00000	
1102	Mg++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	
1103	Mg++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1104	Mg++	PO4=	0.00000	0.00000	0.00000	0.00000	0.00000	
1105	MgOH+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	
1106	MgOH+	SO4=	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+	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1113	MgOH+	B(OH)4(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+	C1O4-	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+	C1-	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+	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1133	H+	B(OH)4(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+	C1O4-	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+	C1-	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+	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1153	MgB(OH)4+	B(OH)4(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+	C1O4-	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+	C1-	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+	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1173	CAB(OH)4+	B(OH)4(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+	C1O4-	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+++	C1-	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+++	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1193	Am+++	B(OH)4(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+++	C1O4-	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+	C1-	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+	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1213	AmCO3+	B(OH)4(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+	C1O4-	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++++	C1-	0.00000	0.00000	0.00000	0.00000		

Appendix J: OUTPUT File Listing of HMW_NP_AM_RTST.CHEMDAT

1231	Th****	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1232	Th****	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1233	Th****	B(OH)2(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---	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++	H2O4-	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++	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1253	UO2++	B(OH)2(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---	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+	H2O4-	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+	B(OH)3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1273	NpO2+	B(OH)2(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---	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

using PITZER ACTIVITY COEFFICIENT model
 Charge Balance replaces element oxygen

this is a BATCH problem

FOR088 file name is U1(SCBARR.FMT.UH)BATCH_DOC_FOR088.1

Ideal Gas Constant is Unity (Dimensionless)
 Temperature = 299.15 [=] 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(VI)	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 H2O4-	H2O4- aqueous	97.066	-304.9420
11 OH-	OH- aqueous	17.007	-83.4350
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 B(OH)3(OH)4-	B(OH)3(OH)4- aqueous	148.457	-963.7700
20 B(OH)2(OH)4*	B(OH)2(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

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)NaNpO2(CO3)2(s)'		
5	2.d3	AmHCO3(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	NaK3(SO4)2	Aphthitalite/Glasserite	
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	2350.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 Tetrahydrate	
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	Geylussite	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	Hexahydrate	
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	Mercurite	
38	1490.d0	Na2SO4.10H2O	Mirabilite	CRC p.B-181:185
39	2.d3	KHS6(SO4)7	Misenerite	
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)4.3H2O	Polyhalite	
46	2.d3	Ca(OH)2	Portlandite	
47	2.d3	K2CO3.3/2H2O	Potassium Carbonate	
48	2.d3	KBH4(CO3)6.3H2O	K-Sequecarbonate	
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	Thénardite	
58	2355.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-Tetaborate (30 C)	
64	2.d3	NaBO2.4H2O	Sodium Metaborate	
65	2.d3	NaB5O8.5H2O	Sodium Pentaborate	
66	2.d3	NaBO2.NaCl.2H2O	Teepelite (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

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1 INPUT file name is:U1:[SCBARS.PWT.UH]BATCH_DOC.IN;1
2 INPUT file name is:U1:[SCBARS.PWT.UH]BATCH_DOC.INGUESS;1
3 OUTPUT file name is:U1:[SCBARS.PWT.UH]BATCH_DOC.OUT;1
4 CHEMIST file name is:U1:[SCBARS.PWT.UH]PWT_PRM_HP_AM_TEST.CHEMIST;1
5 Temperature is Hard Coded as 298.15K
6 [P.D.TITRATE]BATCH_DOC.IN; to illustrate/document "BATCH" runs PWT V2.3
7 DATABASE: HW84/PW86; Np(V)-Na-CO3-OH-Cl-C104 (NR94);
8 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RPFR92,RPF94,RPFF94)
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11 *** ECHO PRINT OF 'CHEMIST' FILE WOULD BE HERE ***
12 *** SEE APPENDIX J ***
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15 Will calculate gamma for B3O3(OH)4- B3O3(OH)4-
16 will calculate gamma for B4O5(OH)4- B4O5(OH)4-
17 will calculate gamma for HCl(aq).....to.titrate.acid.only
18 will calculate gamma for NaOH(aq).....to.titrate.base.only
19
20 *****SOLUBILITY PRODUCT VIOLATION*****
21 ** Mg(OH)2 Brucite ** 1.00E+01 **
22
23 *****SOLUBILITY PRODUCT VIOLATION*****
24 ** MgCl2(OH)3.4H2O MgOxychloride ** 6.69E+00 **
25
26 2 solubility Product Violations
27 Adding solid Mg(OH)2 Brucite
28 # inversions for batch pblm 84
29 [P.D.TITRATE]BATCH_DOC.IN; to illustrate/document "BATCH" runs PWT V2.3
30 DATABASE: HW84/PW86; Np(V)-Na-CO3-OH-Cl-C104 (NR94);
31 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RPFR92,RPF94,RPFF94)
32 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
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Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.10222364E+02	1.11116160E+02	1.10794096E+02	1.11669359E+05	Hydrogen
5.51654402E+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	1.00812732E-03	1.00520523E-03	1.12611601E+03	Magnesium
1.00000000E-04	1.00812732E-04	1.00520523E-04	0.02886254E+00	Calcium
1.00000000E-01	1.00812732E-01	1.00520523E-01	1.92012950E+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	Position
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neofion
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	C104-(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
1.11005846E-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)	10.7462098613920	g/kgH2O

Specified Solution Density

DENSITY	1007.81851904202	kg/m ³ = g/l
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Solution Parameters Based on Specified Density

SOLUTION VOL	0.9946217282285	liters
TDS	10.7170555829390	g/l

Density based on TDS and NaCl solutions 1007.81851904202 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	9.92444E-01	9.93023E-01	1.001	5.50612E+01	5.53476E+01	9.97101E+05	
Na+	2.01625E-01	1.47085E-01	0.7295	2.00000E-01	2.01041E-01	4.62189E+03	
Cl-	1.00813E-01	7.98916E-02	0.7204	1.00000E-01	1.10573E-01	3.93018E+02	
OH-	9.07965E-02	7.13753E-02	0.7224	9.80001E-02	9.85102E-02	1.67519E+03	
K+	1.00813E-02	7.14149E-03	0.7282	1.00000E-02	1.00521E-02	3.93018E+02	
SO4=	1.00813E-03	2.24998E-03	0.2232	1.00000E-03	1.00521E-03	9.65576E+01	
Mg(OH)2	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	0.8566	9.98971E-08	1.00417E-07	7.91480E-03
Mg++	Mg++	1.09873E-08	2.56221E-09	0.2332	1.08988E-08	1.09555E-08	2.66273E-04
MgOH+	MgOH+	3.54268E-08	2.81647E-08	0.7950	3.51412E-08	3.53241E-08	1.45932E-03
MgCO3(aq)	MgCO3(aq)	5.32206E-11	5.32206E-11	1.000	5.27915E-11	5.30663E-11	4.47424E-06
CaCO3(aq)	CaCO3(aq)	6.97236E-07	6.97236E-07	1.000	6.91615E-07	6.95215E-07	6.95835E-02
HCO3-	HCO3-	1.10084E-07	7.49923E-08	0.6812	1.09206E-07	1.09775E-07	6.69815E-03
Mg(OH)4-	Mg(OH)4-	6.18470E-15	4.24905E-15	0.6870	6.13484E-15	6.16677E-15	6.36066E-10
CaB(OH)4-	CaB(OH)4-	8.72370E-11	5.94047E-11	0.6810	8.65337E-11	8.69841E-11	1.03441E-05
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
H+	H+	1.93212E-13	1.40201E-13	0.7256	1.91654E-13	1.92652E-13	1.94173E-10
CO2(aq)	CO2(aq)	2.2143E-14	2.30277E-14	1.041	2.19360E-14	2.20501E-14	9.70422E-10
HCO4-	HCO4-	4.40989E-15	1.00314E-15	0.7382	4.02519E-15	4.05620E-15	1.93717E-10
ESH4(CO3)1.6.H2O	Sequeicarbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
NaBSO8.SHO	Sodium_Pentaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
NaSO2.NaCl.2H2O	Trapsite_20_C	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
CaSO4	Anhydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
NaK3(SO4)2	Aphthalite/Glauberite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
CaCl2.6H2O	Antarcticite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
CaCO3	Aragonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
K2SO4	Arcanite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
MgCl2.6H2O	Bischofite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
Na2Mg(SO4)2.4H2O	Bloedite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00

INFORMATION ONLY

Appendix L: Sample Output File 'BATCH_DOCOUT'

115	Na6CO3 (S04) 2	Burkeite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.61E+01
116	CaCO3	Calcite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.02E-01
117	CaCl2.4H2O	CaCl2 Tetrahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.26E-01
118	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
120	MgCl2.6H2O	Carnallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.84E+01
121	MgSO4.7H2O	Epsomite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.04E+01
122	CaNa2(CO3)2.5H2O	Geyssite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.18E+00
123	CaSO4(SO4)2	Glauberite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.41E+00
124	CaSO4.2H2O	Gypsum	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.77E+00
125	NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.50E+00
126	MgSO4.6H2O	Hexahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.06E+01
127	MgCl2(SO4).3H2O	Kainite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.53E+01
128	K2CO3	Kalicinite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.54E+00
129	MgSO4.H2O	Kilassite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.21E+01
130	K2Mg(SO4)2.4H2O	Isocite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+01
131	Na4Ca(SO4)3.2H2O	Labille Salt	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.33E+01
132	MgCO3	Magnesite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.37E+00
133	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
134	MgSO4	Mercallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.72E+01
135	Na2SO4.10H2O	Mirabilite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.12E+00
136	NaNO2.4H2O	Sodium Nitrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.35E+00
137	NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.55E+00
138	Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.48E+00
139	MgCO3.3H2O	Nesquehonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.04E+00
140	K2Mg(SO4)2.6H2O	Picromarite/Schoen	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.58E+01
141	Na2Ca(CO3)2.2H2O	Piscesonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.35E+00
142	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
143	Ca(OH)2	Portlandite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.80E+00
144	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
145	KNaCO3.6H2O	K-Na Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.48E+00
146	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
147	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
148	Na3H(SO4)2	Sesquisodium Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.18E+01
149	Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.84E+00
150	KCl	Sylvite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.13E+00
151	K2Ca(SO4)2.H2O	Syngonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.82E+00
152	Mg2CaCl6.12H2O	Tachyhydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.59E+01
153	Na2SO4	Thénardite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.03E+00
154	Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.76E+00
155	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
156	Na2B4O7.10H2O	Borax	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.16E+01
157	B(OH)3	Boric Acid Solid	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.08E+01
158	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
159	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
160	KB6(SO4)7	Kisnerite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+02
161	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
162	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
163	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
164	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
165	B3O3(OH)4-	B3O3(OH)4-	0.00000E+00	0.00000E+00	0.3748	0.00000E+00	0.00000E+00	0.00000E+00	-2.70E+01
166	pH (-log[AH+]), pM(-log[m+])		12.8532		12.7140				
167	Osmotic Coefficient=		0.919612						
168	Equilibrium RM (s) =		99.302313						
169	Ionic Strength (m) =		0.213115						
170	Density, Kg/m3 =		1007.82						
171	fCO2(g); log{fCO2(g)}=				6.983E-13			-12.2	
172	NOTES:								
173	- Water "molality" is mole fraction H2O in aqueous phase								
174	- Gas "molality" and "activity" are gas partial pressures								
175	- "Descriptor" means:								
176	*G/RT/ln10 for species with nonzero concs. (convergence criterion)								
177	*Saturation Index for minerals, SI=log10(IAP/Ksp)								
178	*log10(activity) for aqueous species with very small concentrations								
179	*log10(partial pressure) for gases								
180									
181	Total G/RT=		-5.30370149E+03						
182									
183	Total Diagonal Inversions		84						
184	Total Stoichiometric Reoptimizations		9						

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

See Table 15 for explanation of this listing.

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1 INPUT file name is:U1:(SCBABS.FMT.UN)NP_NACL_BM_LOG.IN;1
2 INGRESS file name is:U1:(SCBABS.FMT.UN)NP_NACL_BM_LOG.INGRESS;1
3 OUTPUT file name is:U1:(SCBABS.FMT.UN)NP_NACL_BM_LOG.OUT;1
4 CHEMIST file name is:U1:(SCBABS.FMT.UN)FMT_NHM_NP_AM_STEELT.CHEMIST;1
5 Temperature is Hard Coded as 298.15K
6 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
7 DATABASE: IOM84/FM86; Np(V)-Na-CO3-OH-Cl-C1O4 (NR94);
8 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89, PRF90, P91, RFFR92, RFF94, RFF94)
9
10 Accuracy of reactions is 1.0000E-06
11 Minimum elemental abundance is 1.0000E-18
12 Number of Aqueous Species is 50
13
14 PITER Data Base NOT Echoed in this Run
15
16 Species Order for Pitzer Parameters
17
18 Cations 13
19
20 Na+ K+ Ca++ Mg++ MgOH+ H+
21 MgB(OH)4+ CaB(OH)4+ Am+++ AmCO3+ Th+++ UO2++
22 NpO2+
23
24 Anions 20
25
26 Cl- SO4= HSO4= OH- HCO3- CO3=
27 B(OH)4- B(O3)(OH)4- B(O4)(OH)4= Br- Am(CO3)2- Am(CO3)3--
28 ClO4- pe NpO2(OH)2- NpO2CO3- NpO2(CO3)2+- NpO2(CO3)3--- H2PO4-
29 HPO4= PO4=
30
31 Neutral 6
32
33 CO2(aq) CaCO3(aq) MgCO3(aq) B(OH)3(aq) NpO2OH(aq) H3PO4(aq)
34
35 using PITER ACTIVITY COEFFICIENT model
36 Charge Balance replaces element Oxygen
37
38 this is a TITRATION problem
39
40
41
42
43 Ideal Gas Constant is Unity (Dimensionless)
44 Temperature = 298.15 [=] degree Kelvin
45
46
47
48 115 Species 23 Elements
49
50 Element Name Molecular Weight
51 Hydrogen 1.00790
52 Oxygen 15.99940
53 Sodium 22.98977
54 Potassium 39.09830
55 Magnesium 24.30500
56 Calcium 40.08000
57 Chlorine 35.45300
58 Sulfur 32.06000
59 Carbon 12.01100
60 PosIon 0.00000
61 NegIon 0.00000
62 Air 28.84000
63 Boron 10.81000
64 Bromine 79.90400
65 TracerEl 0.00000
66 Th(IV) 232.03810
67 Am(III) 243.00000
68 U(VI) 238.02900
69 Np(V) 237.04820
70 ClO4-(EL) 99.45060
71 Phosphorus 30.97400
72 Electron 0.00000
73 Charge 0.00000
74
75
76 Species Name Phase Mol.Wt. Std Chemical Potential, u/RT
77 1 H2O WATER aqueous 18.015 -95.6635
78 2 Na+ Na+ aqueous 22.990 -105.6510
79 3 K+ K+ aqueous 39.098 -113.9570
80 4 Ca++ Ca++ aqueous 40.080 -223.1000
81 5 Mg++ Mg++ aqueous 24.305 -183.4680
82 6 MgOH+ MgOH+ aqueous 41.312 -251.9400
83 7 H+ H+ aqueous 1.008 0.0000
84 8 Cl- Cl- aqueous 35.453 -52.9550
85 9 SO4= SO4= aqueous 96.058 -300.3860
86 10 HSO4= HSO4= aqueous 97.066 -304.9420
87 11 OH- OH- aqueous 17.007 -63.4350
88 12 HCO3- HCO3- aqueous 61.017 -236.7510
89 13 CO3= CO3= aqueous 60.009 -212.9440
90 14 CO2(aq) CO2(aq) aqueous 44.010 -155.6800
91 15 CaCO3(aq) CaCO3(aq) aqueous 100.089 -443.5000
92 16 MgCO3(aq) MgCO3(aq) aqueous 84.314 -403.1550
93 17 B(OH)3(aq) B(OH)3(aq) aqueous 61.832 -390.8100
94 18 B(OH)4- B(OH)4- aqueous 78.839 -465.2000
95 19 B(O3)(OH)4- B(O3)(OH)4- aqueous 148.457 -963.7700
96 20 B(O4)(OH)4= B(O4)(OH)4= aqueous 191.266 -1239.1000
97 21 CaB(OH)4+ CaB(OH)4+ aqueous 118.919 -692.1000
98 22 MgB(OH)4+ MgB(OH)4+ aqueous 103.144 -651.8900
99 23 Br- Br- aqueous 79.904 -399.9900
100 24 ClO4- perchlorate ClO4- aqueous 99.451 -399.9900
101 25 NaOH(aq).....to.titrate.base.only aqueous 39.997 500.0000
102 26 HCl(aq).....to.titrate.acid.only aqueous 36.461 500.0000
103 27 HClO4(aq).....to.titrate.acid.only aqueous 100.459 500.0000
104 28 PosIon.....POSITIVE ION aqueous 0.000 0.0000
105 29 NegIon.....NEGATIVE ION aqueous 0.000 0.0000
106 30 PosIon(OH)(aq).....to.titrate.base aqueous 17.007 500.0000
107 31 HNegIon(aq).....to.titrate.acid aqueous 1.008 500.0000
108 32 Tracer(aq).....conservative.tracer aqueous 0.000 0.0000
109 33 H3PO4(aq) H3PO4(aq) aqueous 97.995 -460.9000
110 34 H2PO4- H2PO4- aqueous 96.987 -455.9600
111 35 HPO4= HPO4= aqueous 95.980 -439.3670
112 36 PO4= PO4= aqueous 94.972 -410.9470
113 37 NpO2+ NpO2+ aqueous 269.047 -369.1270
114 38 NpO2OH(aq) NpO2OH(aq) aqueous 286.054 -438.5180
115 39 NpO2(OH)2- NpO2(OH)2- aqueous 303.062 -505.8390

```


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	8.57464E-01	8.59843E-01	1.001	5.55025E+01	5.00446E+01	9.01564E+05	
Na+	5.61062E+00	3.69881E+00	0.6593	5.61000E+00	5.05833E+00	1.16290E+05	
CO3=	1.99407E+00	4.09214E-02	2.0522E-02	1.99185E+00	1.79778E+00	1.07884E+05	
Cl-	1.61018E+00	1.06477E+00	0.6613	1.61000E+00	1.45165E+00	5.14664E+04	
HCO3-	6.14733E-03	1.59044E-03	0.2587	6.14665E-03	5.54221E-03	9.42508E+01	2.07E-11
OH-	6.14733E-03	4.86901E-03	0.7921	6.14665E-03	5.54221E-03	9.42508E+01	
CO2(aq)	2.16876E-09	7.15913E-09	3.022	2.16850E-09	2.13559E-09	9.39668E-05	-2.10E-07
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	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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.30E-02
Na2CO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.95E-01
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.51E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.83E+00
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.57E+00

pH (-log(aH+)) ; pOH(-log(aOH-)) 11.7497 11.6199
 Osmotic Coefficient= 0.908416
 Equilibrium RM (s) = 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:
 *G/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+01

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

shifting left by 4.64434654478256
 calling makemuv for allomorphic reactions
 # inversions for batch plm 99

Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.1

DATA BASE: RHW4/PWB; Np(V)O2-CO3-Cl-C104 (R94);
 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (RFRS89, RFR90, RFR91, RFR92, RFR94, RFR99)

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	9.91838668E+01	1.00169020E+05	Hydrogen
1.05508682E+02	5.55113597E+01	4.96942389E+01	7.95078006E+03	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	5.02297775E+00	1.78079701E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
1.00000000E+01	6.12839260E-04	5.48618692E-04	6.58946151E+00	Carbon
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	Mercury
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	5.48618692E-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) 328.108912108174 g/kgH2O
 Specified Solution Density 1188.93254605458 kg/m3 = g/l
 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 0.00000000000000E+00 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.11822E-01	7.77959E-01	0.9352	5.55091E+01	4.96910E+01	8.95208E+05	
Na2NpO2CO3(s)	3.99932E+00	1.00000E+00	1.000	9.99939E+00	8.95147E+00	3.15133E+06	
Cl-	5.61057E+00	5.29268E+00	0.9433	5.61000E+00	5.02263E+00	1.15469E+05	
NpO2+	6.12705E-04	1.21978E-03	1.991	6.12709E-04	5.48499E-04	1.47572E+02	
CO2(aq)	3.86103E-04	1.12115E-03	2.904	3.86106E-04	3.45643E-04	1.52117E+01	
HCO3-	2.26571E-04	8.38010E-05	0.3702	2.26573E-04	2.02829E-04	1.23760E+01	1.23E-14
H+	1.21872E-06	4.78095E-06	3.923	1.21873E-06	1.09101E-06	1.09962E-03	1.23E-14
NpO2CO3-	1.33246E-07	2.42971E-07	1.820	1.33247E-07	1.19548E-07	1.93334E-02	1.85E-14
CO3=	3.09384E-08	8.03343E-10	2.5966E-02	3.09386E-08	2.76963E-08	1.66203E-03	0.00E+00
OH-	3.01685E-09	1.63977E-09	0.5435	3.01687E-09	2.70071E-09	4.59318E-05	1.23E-14
NpO2OH(aq)	7.72186E-10	1.72186E-10	1.000	7.72191E-10	6.91267E-10	1.97740E-04	-6.17E-15
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-	2.04381E-16	6.10703E-17	0.2988	2.04383E-16	1.82964E-16	5.54494E-11	0.00E+00
NpO2(CO3)3=	1.25197E-16	9.87897E-26	7.8908E-10	1.25198E-16	1.12077E-16	5.03110E-11	-2.25E-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)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+00
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.24E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.95E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.91E+00
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+00
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
Na3NpO2(CO3)2(n)_DISABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.36E+02
NpO2OH(saged)	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"

```

487 pH (-log(aH+)); pOH(-log(mH+))      5.3205      5.9141
488 Osmotic Coefficient= 1.241871
489 Equilibrium RM (#) = 77.795863
490 Ionic Strength (m) = 5.611188
491 Density, kg/m3 = 1188.93
492 fCO2(g); log(fCO2(g))= 3.400E-02 -1.47
493
494 NOTES: - Water "molarity" is mole fraction H2O in aqueous phase
495         - Gas "molarity" and "activity" are gas partial pressures
496         - "Descriptor" means:
497           *dq/RT*ln10 for species with nonzero concs. (convergence criterion)
498           *Saturation Index for minerals, SI=log10(IAP/Ksp)
499           *log10(activity) for aqueous species with very small concentrations
500           *log10(partial pressure) for gases
501
502 Total G/RT= -1.3323084E+04
503 Flashing Titration # 1
504 # inversions for batch pbln 17
505
506 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO2 in 5.61molal NaCl FWT V2.3
507 DATABASE: BSM84/PW86; Np(V)-Na-CO3-OH-Cl-C1O4 (BS94);
508 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRS85,FRP90,P91,RFFR92,RFF94,RFF94)
509 Pressure= 1.00000E+00 (=) ATM Temperature= 2.985E+02 (=) Kelvin
510
511 Elemental Abundances for Flash Problem

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Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1.85857174E+01	1.11017591E+02	9.93838868E+01	1.00169020E+05	Hydrogen
1.66707638E+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	5.02237975E+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	U(VI)
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	TracerCl
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	1.00049118E+02	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	C1O4-(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

```

512 Solution Parameters, Calculated
513 SOLUTION MASS 461.602144251003 grams
514 H2O MASS 347.563995068949 grams
515 TDS(g/kg) 328.106912108174 g/kgGO
516
517 Specified Solution Density 1188.93254605458 kg/m3 = g/l
518
519 Solution Parameters Based on Specified Density
520 SOLUTION VOL 0.388249228926239 liters
521 TDS 293.724084133903 g/l
522
523 Density based on TDS and NaCl solutions 1188.93254605458 g/l
524 Percent relative error vs NaCl density 0.00000000000000E+00 %

```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31822E-01	7.77959E-01	0.9352	1.92928E+01	4.96918E+01	8.95208E+05	
Na2O2CO3(s)	9.99932E+00	1.00000E+00	1.0000	3.47540E+00	8.95147E+00	3.15133E+06	
Cl-	5.61096E+00	5.29329E+00	0.9434	1.95017E+00	5.02298E+00	1.78080E+05	
Na+	5.61057E+00	5.29268E+00	0.9433	1.95003E+00	5.02263E+00	1.75469E+05	
NpO2+	6.12295E-04	1.21978E-03	1.991	2.12954E-04	5.48649E-04	1.47572E+02	
CO2(aq)	3.86103E-04	1.12115E-03	2.904	1.34196E-04	3.45643E-04	1.52117E+01	
HCO3-	2.26571E-04	0.38810E-05	0.3702	7.87481E-05	2.02829E-04	1.23760E-01	-5.15E-12
H+	1.21872E-06	4.78095E-06	3.923	4.23582E-07	1.09101E-06	1.09962E-03	-2.29E-11
NpO2CO3-	1.33526E-07	2.42971E-07	1.820	4.64090E-08	1.19534E-07	3.93334E-02	1.85E-14
CO3=	3.09384E-08	8.03343E-10	2.5966E-02	1.07531E-08	2.76963E-08	1.66203E-03	1.68E-11
OH-	3.01639E-08	1.63977E-09	0.5435	1.04855E-09	2.70071E-09	4.59318E-05	2.30E-11
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=	1.98384E-11	5.13355E-16	2.5877E-05	6.89511E-12	1.77595E-11	6.90960E-06	1.69E-11
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=	1.25197E-16	9.87897E-26	7.8908E-10	4.35139E-17	1.12077E-16	5.03310E-11	-3.15E-10
HCl(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.45E+02
NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.24E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.95E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.91E+00
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+00
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.16E+02
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+00
NpO2OH(aq)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.38E+00

```

557 pH (-log(aH+)); pOH(-log(mH+))      5.3205      5.9141
558 Osmotic Coefficient= 1.241871
559 Equilibrium RM (#) = 77.795863
560 Ionic Strength (m) = 5.611188
561 Density, kg/m3 = 1188.93
562 fCO2(g); log(fCO2(g))= 3.400E-02 -1.47
563
564 NOTES: - Water "molarity" is mole fraction H2O in aqueous phase
565         - Gas "molarity" and "activity" are gas partial pressures
566         - "Descriptor" means:
567           *dq/RT*ln10 for species with nonzero concs. (convergence criterion)
568           *Saturation Index for minerals, SI=log10(IAP/Ksp)
569           *log10(activity) for aqueous species with very small concentrations
570           *log10(partial pressure) for gases
571
572 Total G/RT= -4.6337981E+03
573 Flashing Titration # 2
574 # inversions for batch pbln 19
575
576 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO2 in 5.61molal NaCl FWT V2.3
577 DATABASE: BSM84/PW86; Np(V)-Na-CO3-OH-Cl-C1O4 (BS94);
578 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRS85,FRP90,P91,RFFR92,RFF94,RFF94)
579 Pressure= 1.00000E+00 (=) ATM Temperature= 2.985E+02 (=) Kelvin
580
581 Elemental Abundances for Flash Problem

```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

	Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
611					
612					
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+05	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	5.02231443E+00	1.78056128E+05	Chlorine
621	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
622	3.47579611E+00	6.30932337E-04	6.18560128E-04	7.42952570E+00	Carbon
623	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Poison
624	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Helion
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	1.54179448E-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	-1.92287521E-15	-3.51197080E-15	0.00000000E+00	Charge

Solution Parameters, Calculated
 SOLUTION MASS 461.665999617212 grams
 H2O MASS 347.6536756849709 grams
 TDS(g/kg) 327.947988724245 g/kgH2O

Specified Solution Density
 DENSITY 1188.85111378691 kg/m³ = 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 1188.85111378691 g/l
 Percent relative error vs NaCl density 0.000000000000000000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	0.31845E-01	7.78011E-01	0.9353	1.92978E+01	4.96944E+01	8.95254E+05	
NaHPO2(CO3) (a)	9.99718E+00	1.00000E+00	1.000	3.47556E+00	8.95002E+00	2.15082E+06	
Na+	5.61014E+00	5.29140E+00	0.9432	1.95039E+00	5.02250E+00	1.15466E+05	
Cl-	5.60993E+00	5.29133E+00	0.9432	1.95031E+00	5.02231E+00	1.78056E+05	
NaCO3-	3.82212E-00	0.41513E-04	0.3702	1.32878E-04	3.42117E-04	2.08787E-01	
CO2(aq)	3.08476E-04	8.95671E-04	2.904	1.07243E-04	2.76165E-04	1.21539E+01	
NpO2+	1.72085E-04	3.42461E-04	1.990	5.98256E-05	1.54059E-04	4.14492E+01	-1.82E-10
H+	5.77346E-07	2.26410E-06	3.922	2.00716E-07	5.16872E-07	5.20955E-04	-2.18E-10
NpO2CO3-	1.33573E-07	2.43030E-07	1.619	4.64370E-08	1.19581E-07	3.93490E-02	8.02E-14
CO3=	1.10193E-07	2.86188E-09	2.5971E-02	3.83099E-08	9.86531E-08	5.92010E-03	3.31E-10
OH-	6.37029E-09	3.46282E-09	0.5436	2.21466E-09	5.70303E-09	9.69912E-05	2.19E-10
NpO2OH(aq)	4.57851E-10	4.57851E-10	1.000	1.59174E-10	4.09893E-10	1.17252E-04	-1.34E-10
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=	1.58546E-15	1.25405E-24	7.9097E-10	5.51192E-16	1.41939E-15	6.37413E-10	5.26E-10
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	-2.43E+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)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.61E+00
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.21E+00
NaHNP02(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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E+01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.72E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.36E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.48E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.69E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.40E+00

pH (-log[OH-]); pOH(-log[OH-]) 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:
 *G/R/T/ln/0 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/R/T= -4.63438031E+03
 Flashing Titration # 3
 # inversions for batch phis 28
 1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO2 in 5.61molal NaCl PWT V2.3
 DATABASE: RM84/RM86; Np(V)-Na-CO3-OH-Cl-O4 (RM84);
 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (RPM89, RPF90, P91, RPF92, RPF94, RPF94)
 707 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
710				
711				
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+05 Oxygen
715	5.42615710E+00	5.61002379E+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	5.60950151E+00	5.02199808E+00	1.78044899E+05 Chlorine
720	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Sulfur
721	3.47587277E+00	7.30126088E-04	7.07373490E-04	8.49626299E+00 Carbon
722	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Poison
723	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Helion
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	5.09860080E-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"

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735 -2.11316242E-15 -6.07769560E-15 -5.44115783E-15 0.00000000E+00 Charge
736
737 Solution Parameters, Calculated
738 SOLUTION MASS 461.701224245767 grams
739 H2O MASS 347.691387660714 grams
740 TDS (g/kg) 327.905264930827 g/kgH2O
741
742 Specified Solution Density
743 DENSITY 1188.82922071360 kg/m3 = g/l
744
745 Solution Parameters Based on Specified Density
746 SOLUTION VOL 0.388366315532375 liters
747 TDS 293.562628954490 g/l
748
749 Density based on TDS and NaCl solutions 1188.82922071360 g/l
750 Percent relative error vs NaCl density 0.000000000000000E+000 %
751
752
753
754
755

```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31852E-01	7.78030E-01	0.9353	1.92999E+01	4.96951E+01	8.95267E+05	
NaHPO2CO3(s)	9.99622E+00	1.00000E+00	1.000	3.47562E+00	8.94928E+00	3.15056E+06	
Na+	5.61603E+00	5.29080E+00	0.9431	1.95056E+00	5.02247E+00	1.15465E+05	
Cl-	5.60952E+00	7.72603E-09	0.9436	1.95037E+00	5.02200E+00	1.17804E+05	
HCO3-	5.79855E-04	2.14695E-04	0.3703	2.01612E-04	5.19125E-04	1.16755E+01	
CO2(aq)	2.09763E-04	6.09044E-04	2.903	7.29329E-05	1.87794E-04	8.26478E+00	
NpO2+	5.08519E-05	1.01191E-04	1.990	1.76808E-05	4.55260E-05	1.22486E+01	-1.83E-10
CO3=	3.72979E-07	9.68710E-09	2.5972E-02	1.29642E-07	3.33916E-07	2.00380E-02	-1.16E-10
H+	2.58813E-07	1.01480E-06	3.921	8.99871E-08	2.31707E-07	2.33537E-04	-1.00E-10
NpO2CO3-	1.13591E-07	2.43057E-07	1.819	4.64488E-08	1.19600E-07	2.93550E-02	3.70E-14
OH-	1.42123E-08	7.72603E-09	0.5436	4.94149E-09	1.27238E-08	2.16397E-04	1.02E-10
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=	2.39201E-10	6.19248E-15	2.5888E-05	8.31683E-11	2.14148E-10	8.33180E-05	1.24E-10
NpO2(CO3)3=	1.81540E-14	1.43698E-23	7.9155E-10	6.31199E-15	1.62527E-14	7.29866E-09	-3.61E-11
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)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.45E+02
NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+02
NpO2OH(aqsd)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.39E+00
NpO2OH(amor)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.35E+02
NaHPO2(CO3)2(s)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.54E+00
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.83E+00
Na2CO3 10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.87E+00
Na2CO3 7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.16E+00
Na2CO3 H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.68E+00
NaH(CO3)2 2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	

```

756 pH (-log(aH+)); pOH (-log(aOH)) 5.9936 6.5870
757 Osmotic Coefficient= 1.241881
758 Equilibrium RM (%) = 77.803013
759 Ionic strength (m) = 5.610081
760 Density, kg/m3 = 1188.83
761 fCO2(g); log(fCO2(g))= 1.647E-02 -1.73
762
763 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
764 - Gas "molality" and "activity" are gas partial pressures
765 - "Descriptor" means:
766 * "O/RT/ln10" for species with nonzero concs. (convergence criterion)
767 * "Saturation Index for minerals, SI=log10(IAP/Ksp)
768 * "log10(activity)" for aqueous species with very small concentrations
769 * "log10(partial pressure)" for gases

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800 Total G/RT= -4.63462770E+03
801 Flashing Titration # 4
802 # inversions for batch pbm 20
803 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO2 in 5.61molar NaCl FMT V1.3
804 DATABASE: H2O/NaCl; Np(V)-Na-CO3-OH-Cl-C104 (DR94);
805 95.01.33 Am(III)-Na-Cl-CO3-204-P04 (FUSRES, RFF70, P91, RFFRS2, RFF74, RFF79)
806 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
807
808 Elemental Abundances for Flash Problem
809
810 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
811 3.86060470E+01 1.11018357E+02 9.93815462E+01 1.00176739E+05 Hydrogen
812 2.66820273E+01 5.55118409E+01 4.96981566E+01 7.95140687E+05 Oxygen
813 5.42646354E+00 5.61000023E+00 5.02247206E+00 1.15465478E+05 Sodium
814 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
815 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
816 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
817 1.9504284E+00 5.6088928E+00 5.02148063E+00 1.78024553E+05 Chlorine
818 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
819 3.47598202E+00 1.05369370E-03 9.43341702E-04 1.13304772E+01 Carbon
820 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
821 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Nitrogen
822 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron
823 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bromine
824 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Strontium
825 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Thallium
826 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Lead
827 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bismuth
828 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Antimony
829 3.47561578E+00 5.04731448E-07 4.51871568E-07 1.07115142E-01 Np(V)
830 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Np(IV)
831 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Np(III)
832 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Np(II)
833 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Electron
834 -1.15000139E-15 -3.30702765E-15 -2.96068686E-15 0.00000000E+00 Charge
835
836 Solution Parameters, Calculated
837 SOLUTION MASS 461.746388131807 grams
838 H2O MASS 347.7447153531108 grams
839 TDS (g/kg) 327.889016696973 g/kgH2O
840
841 Specified Solution Density
842 DENSITY 1188.82089442743 kg/m3 = g/l
843
844 Solution Parameters Based on Specified Density
845 SOLUTION VOL 0.388423849459851 liters
846 TDS 293.5495618380179 g/l
847
848 Density based on TDS and NaCl solutions 1188.82089442743 g/l
849 Percent relative error vs NaCl density 0.000000000000000E+000 %
850
851
852
853
854

```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31857E-01	7.78050E-01	0.9353	1.93029E+01	4.96953E+01	8.95271E+05	
NaHPO2CO3(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"

859	Na+	Na+	5.61000E+00	5.29000E+00	0.9430	1.95005E+00	5.02247E+00	1.15465E+05
860	Cl-	Cl-	5.60889E+00	5.28992E+00	0.9421	1.95046E+00	5.02148E+00	1.15465E+05
861	HCO3-	HCO3-	9.92460E-04	1.67543E-04	0.1703	1.45192E-04	8.88700E-04	5.42959E+01
862	CO3=	CO3=	5.67888E-05	1.47494E-06	2.5972E-02	1.97480E-05	5.08414E-05	3.05095E+00
863	CO2(aq)	CO2(aq)	4.03745E-06	1.17227E-05	2.903	1.40400E-06	3.61461E-06	1.59078E-01
864	OH-	OH-	1.26397E-06	6.87170E-07	0.5437	4.39540E-07	1.13160E-06	1.92454E-02
865	HPO2-	HPO2-	3.14101E-07	6.64703E-07	1.990	1.16182E-07	2.39111E-07	8.04750E-02
866	HPO2CO3-	HPO2CO3-	1.13611E-07	2.43094E-07	1.819	4.64631E-08	1.19430E-07	3.93616E-02
867	HPO2(CO3)2--	HPO2(CO3)2--	3.64205E-08	9.43001E-11	2.5882E-05	1.26650E-08	3.26042E-08	1.132E-07
868	H+	H+	2.91045E-09	1.14100E-08	3.920	1.01214E-09	2.60582E-09	2.62641E-06
869	HPO2(CO3)3===	HPO2(CO3)3===	4.20660E-10	3.33181E-19	7.9204E-10	1.46282E-10	3.76605E-10	1.69124E-04
870	HPO2OH(aq)	HPO2OH(aq)	1.76139E-10	1.76139E-10	1.000	6.13211E-11	1.57872E-10	4.51598E-05
871	HPO2(OH)2-	HPO2(OH)2-	1.95583E-14	5.88438E-15	0.2988	6.80128E-15	1.75100E-14	5.30660E-09
872	HCl(aq).....to.titrate.acid.only	HCl(aq).....to.titrate.acid.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
873	NaOH(aq).....to.titrate.base.only	NaOH(aq).....to.titrate.base.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
874	HPO2OH(aged)	HPO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
875	HPO2OH(amor)	HPO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
876	Na3HPO2(CO3)2(s)_DISABLED_DISABLED	Na3HPO2(CO3)2(s)_DISABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
877	NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
878	NaHCO3	NaHcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
879	Na2CO3.10H2O	Na2tron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
880	Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
881	Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
882	Na3H(CO3)2.2H2O	Troca	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00

pH (-log(aH+)); pOH (-log(aOH+)) 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:
 *O/R/T/ln10 for species with nonzero concn. (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= -4.61497997E+03
 Flashing Titration # 5
 # Inversions for batch pblm 22
 Benchmark TITRATE process, LOG10 option; Hp(V)O2 with CO2 in 5.61molar NaCl PWT V2.3
 DATABASE: IHW84/PW86; Hp(V)-Na-CO3-OH-Cl-ClO4 (HW84);
 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (IFR84,FR90,PP1,RPFR92,RP94,RRF94)
 Pressure= 1.00000E+00 [w] ATM Temperature= 2.98E+02 [w] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1.86146891E+01	1.11018383E+02	9.93917155E+01	1.00176910E+05	Hydrogen
3.66868155E+01	5.55113161E+01	4.96994430E+01	7.95161268E+01	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	5.60799182E+00	5.02068795E+00	1.7799450E+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	Phosphorus
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	Al
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)
1.4757878E+00	5.1843081E+07	4.64127943E+07	1.10220493E+01	Hp(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
-1.62616037E-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 1188.81855435140 kg/m3 = 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 1188.81855435140 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	8.31862E-01	7.78067E-01	0.9353	1.93072E+01	4.96994E+01	8.95273E+05	
Na3HPO2CO3(s)	9.99250E+00	1.00000E+00	1.000	3.47562E+00	8.94601E+00	3.14941E+06	
Na+	5.61000E+00	5.28971E+00	0.9429	1.95128E+00	5.02248E+00	1.15466E+05	
Cl-	5.60889E+00	5.28867E+00	0.9411	1.95059E+00	5.02069E+00	1.15466E+05	
HCO3-	1.00903E-03	1.73572E-04	0.1702	3.50963E-04	9.0356E-04	5.51202E+01	
CO3=	4.90717E-04	1.27445E-05	2.5971E-02	1.70682E-04	4.39325E-04	2.61636E+01	
OH-	1.07447E-05	5.84190E-06	0.5437	1.73726E-06	9.61946E-06	1.63601E-01	-4.54E-08
CO2(aq)	4.82702E-07	1.40153E-06	2.904	1.67895E-07	4.32150E-07	1.90188E-02	-8.59E-08
HPO2(CO3)2--	3.14571E-07	8.14859E-12	2.5904E-05	1.09415E-07	2.81627E-07	1.09571E-01	2.57E-08
HPO2CO3-	1.13610E-07	2.43107E-07	1.819	4.64794E-08	1.19635E-07	1.93666E-02	4.47E-12
H+	3.68807E-08	7.69314E-08	1.985	1.34540E-08	3.48298E-08	9.11704E-03	-1.12E-08
HPO2(CO3)3===	3.13656E-08	2.48770E-17	7.9313E-10	1.09097E-08	2.80808E-08	1.26104E-02	4.46E-08
H+	3.42512E-10	1.34216E-09	3.919	1.19134E-10	3.06642E-10	3.09064E-07	-2.53E-08
HPO2OH(aq)	1.73507E-10	1.73507E-10	1.000	6.03495E-11	1.55316E-10	4.44344E-05	4.67E-09
HPO2(OH)2-	1.62614E-13	4.88873E-14	0.2988	5.6985E-14	1.46479E-13	4.43211E-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
HPO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
HPO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.63E+00
Na3HPO2(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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.71E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.75E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.04E+00
Na3H(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.33E+00

INFORMATION ONLY

FMT, Version 2.3
User's Manual, Version 1.1

WPO # 43037
January 9, 1997
Page 152

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

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983 pH (-log(aH+)), pOH(-log(aOH-))      8.8722      9.4653
984 Osmotic Coefficient= 1.24539
985 Equilibrium RH (%) = 77.806749
986 Ionic Strength (m) = 5.610494
987 Density, kg/m3 = 1188.82
988 fCO2(g); log(fCO2(g))= 4.250E-05 -4.37
989
990 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
991         - Gas "molality" and "activity" are gas partial pressures
992         - "Descriptor" means:
993           *DG/RT/ln10 for species with nonzero concs. (convergence criterion)
994           *Saturation Index for minerals, SI=log10(IAP/Ksp)
995           *log10(activity) for aqueous species with very small concentrations
996           *log10(partial pressure) for gases
997
998 Total Q/RT= -4.63548129E+03
999 Flashing Titration # 6
1000 # inversions for batch pbm 23
1001 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
1002 DATABASE: HMR84/PW86; Np(V)-Na-CO3-OH-Cl-C1O4 (HR84);
1003 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (PFR89,FRF90,P91,RFFR92,RFF94,RFF94)
1004 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
1005
1006 Elemental Abundances for Flash Problem
1007
1008 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
1009
1010 3.86270051E+01 1.11018410E+02 9.2919460E+01 1.00177142E+05 Hydrogen
1011 1.66936391E+01 5.55151239E+01 4.97012721E+01 7.95190533E+05 Oxygen
1012 5.42752260E+00 5.61000344E+00 5.02249276E+00 1.15465953E+05 Sodium
1013 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1014 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
1015 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
1016 1.95076678E+00 5.60825792E+00 5.03955815E+00 1.77358403E+05 Boron
1017 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1018 3.47635958E+00 2.13880634E+03 1.91481868E+03 2.29988871E+01 Carbon
1019 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1020 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Nitrogen
1021 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Air
1022 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Neon
1023 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bromine
1024 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 TracerEl
1025 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Th(IV)
1026 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Am(III)
1027 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 U(VI)
1028 3.47561578E+00 1.62583515E+06 9.18404325E+07 2.17765032E+01 Np(V)
1029 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Cl(aq)
1030 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1031 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Electron
1032 -3.21308874E-15 -3.77396651E-15 -3.37673581E-15 0.00000000E+00 Charge
1033
1034 Solution Parameters, Calculated
1035 SOLUTION MASS 462.013014691130 grams
1036 H2O MASS 347.93330580296 grams
1037 TDS(g/kg) 327.877998698106 g/kgH2O
1038
1039 Specified Solution Density
1040 DENSITY 1188.81524828657 kg/m^3 = g/l
1041
1042 Solution Parameters Based on Specified Density
1043 SOLUTION VOL 0.388633149984595 liters
1044 TDS 293.540795775029 g/l
1045
1046 Density based on TDS and NaCl solutions 1188.81524828657 g/l
1047 Percent relative error vs NaCl density 0.000000000000000000 %
1048
1049
1050
1051 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1052
1053 Species Name Molality Activity Act Coef Total Moles Molarity mg/liter Descriptor
1054
1055 H2O WATER 8.11870E-01 7.78092E-01 0.9354 1.93133E+01 4.96955E+01 8.95274E+05
1056 NaHPO2CO3(s) NaHPO2CO3(s) 9.98931E+00 1.00000E+00 1.000 1.47562E+00 8.94318E+00 1.14861E+06
1057 Na+ Na+ 5.61000E+00 5.28932E+00 0.9428 1.95191E+00 5.02249E+00 1.15466E+05
1058 Cl- Cl- 5.60473E+00 5.28679E+00 0.9429 1.95077E+00 5.01956E+00 1.17795E+05
1059 CO2 CO2 1.11398E-03 2.89293E-05 2.5959E-02 3.87591E-04 9.97318E-04 5.98482E-01
1060 HCO3- HCO3- 1.02256E-03 1.78516E-04 0.3702 3.55784E-04 9.15475E-04 5.58596E-01
1061 OH- OH- 2.40684E-05 1.30877E-05 0.5438 8.37419E-06 2.15478E-05 3.66470E-01 -4.77E-09
1062 NpO2(CO3)2(aq) NpO2(CO3)2(aq) 7.13649E-07 1.84936E-11 2.5921E-05 2.48302E-07 6.38912E-07 2.48578E-01 9.86E-09
1063 CO2(aq) CO2(aq) 2.18328E-07 6.33927E-07 2.904 7.59637E-08 1.95464E-07 6.60232E-03 -2.55E-08
1064 NpO2(CO3)3(aq) NpO2(CO3)3(aq) 1.61312E-07 1.28193E-16 7.9469E-10 5.61257E-08 1.44418E-07 6.48546E-02 1.95E-08
1065 NpO2CO3- NpO2CO3- 1.33654E-07 2.43125E-07 1.819 4.65026E-08 1.19657E-07 3.92738E-02 1.56E-12
1066 NpO2- NpO2- 1.70494E-08 3.38938E-08 1.988 5.93207E-09 1.52639E-08 4.10671E-03 -9.08E-09
1067 NpO2OH(aq) NpO2OH(aq) 1.71249E-10 1.71249E-10 1.000 5.95833E-11 1.53315E-10 4.38564E-05 1.05E-08
1068 H+ H+ 1.52979E-10 5.99129E-10 3.916 5.32265E-11 1.36958E-10 1.38040E-07 -1.95E-08
1069 NpO2(OH)2- NpO2(OH)2- 3.61806E-13 1.08095E-13 0.2988 1.25884E-13 3.23915E-13 9.81662E-08 3.00E-08
1070 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
1071 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
1072 NpO2OH(saged) NpO2OH(saged) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.04E+00
1073 NpO2OH(amor) NpO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.63E+00
1074 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
1075 NaCl Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.24E+01
1076 NaHCO3 NaHCO3 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.30E+00
1077 Na2CO3.10H2O Na2CO3.10H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.16E+00
1078 Na2CO3.7H2O Na2CO3-Heptahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.19E+00
1079 Na2CO3.H2O Thronnatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.68E+00
1080 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
1081
1082 pH (-log(aH+)), pOH(-log(aOH-))      9.2225      9.8154
1083 Osmotic Coefficient= 1.24531
1084 Equilibrium RH (%) = 77.809217
1085 Ionic Strength (m) = 5.611121
1086 Density, kg/m3 = 1188.82
1087 fCO2(g); log(fCO2(g))= 1.922E-05 -4.72
1088
1089 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1090         - Gas "molality" and "activity" are gas partial pressures
1091         - "Descriptor" means:
1092           *DG/RT/ln10 for species with nonzero concs. (convergence criterion)
1093           *Saturation Index for minerals, SI=log10(IAP/Ksp)
1094           *log10(activity) for aqueous species with very small concentrations
1095           *log10(partial pressure) for gases
1096
1097 Total Q/RT= -4.63619544E+03
1098 Flashing Titration # 7
1099 # inversions for batch pbm 23
1100 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
1101 DATABASE: HMR84/PW86; Np(V)-Na-CO3-OH-Cl-C1O4 (HR84);
1102 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (PFR89,FRF90,P91,RFFR92,RFF94,RFF94)
1103 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
1104
1105 Elemental Abundances for Flash Problem
1106
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter					
1107								
1108								
1109	3.86445565E+01	1.11018446E+02	9.93227212E+01	1.00177470E+05 Hydrogen				
1110	3.67033634E+01	5.55178692E+01	4.97038762E+01	7.95231975E+05 Oxygen				
1111	5.42840953E+00	5.61000623E+00	5.02251004E+00	1.15466351E+05 Sodium				
1112	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Potassium				
1113	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Magnesium				
1114	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Calcium				
1115	1.95102131E+00	5.60491242E+00	5.01794966E+00	1.77901699E+05 Chlorine				
1116	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Sulfur				
1117	3.47667578E+00	3.04711826E-03	2.72801516E-03	3.27661900E+01 Carbon				
1118	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 PosIon				
1119	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 NegIon				
1120	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Alf				
1121	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Boron				
1122	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Bromine				
1123	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 TracerEl				
1124	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Th(IV)				
1125	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Am(III)				
1126	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 U(VI)				
1127	3.47561578E+00	1.94421849E-06	1.74061427E-06	4.12609479E-01 Np(V)				
1128	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Np(V)				
1129	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 ClO4-(EL)				
1130	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Phosphorus				
1131	-2.12321556E-15	-6.09959368E-15	-5.46082646E-15	0.00000000E+00 Electron				
1132				0.00000000E+00 Charge				
1133	Solution Parameters, Calculated							
1134	SOLUTION MASS	462.219612785907	grams					
1135	H2O MASS	348.091311120332	grams					
1136	TDS(g/kg)	327.868860898173	g/kgH2O					
1137								
1138	Specified Solution Density							
1139	DENSITY	1188.81056561769	kg/m ³ = g/l					
1140								
1141	Solution Parameters Based on Specified Density							
1142	SOLUTION VOL	0.388808466339415	liters					
1143	TDS	293.533478681879	g/l					
1144								
1145	Density based on TDS and NaCl solutions	1188.81056561769	g/l					
1146	Percent relative error vs NaCl density	0.00000000000000E+000	%					
1147								
1148								
1149								
1150	TABLE OF CONCENTRATIONS FOR BATCH SYSTEM							
1151								
1152	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
1153								
1154	H2O	WATER	8.31881E-01	7.78127E-01	0.9354	1.93221E+01	4.96957E+01	8.95277E+05
1155	NaH2PO4(CO3)(s)	NaH2PO4(CO3)(s)	9.98478E+00	1.00000E+00	1.0000	3.47562E+00	8.93914E+00	3.14699E+06
1156	Na+	Na+	5.61001E+00	5.28876E+00	0.9427	1.95279E+00	5.02251E+00	1.15466E+05
1157	Cl-	Cl-	5.60491E+00	5.28611E+00	0.9428	1.95102E+00	5.01795E+00	1.77901E+05
1158	CO3=	CO3=	2.00203E-03	5.19857E-05	2.5967E-02	6.94883E-04	1.79236E-03	1.07558E+02
1159	HCO3-	HCO3-	1.04073E-03	3.85192E-04	0.3701	3.62268E-04	9.31738E-04	5.68519E+01
1160	OH-	OH-	4.24988E-05	2.31125E-05	0.5438	1.47935E-05	3.80482E-05	6.47098E-01
1161	NpO2(CO3)2=	NpO2(CO3)2=	1.28137E-06	3.32447E-11	2.5945E-05	4.46032E-07	1.14718E-06	4.46327E-01
1162	NpO2(CO3)3=	NpO2(CO3)3=	5.19502E-07	4.13999E-16	7.9692E-10	1.80834E-07	4.65098E-07	2.08864E-01
1163	NpO2CO3-	NpO2CO3-	1.33688E-07	2.43151E-07	1.819	4.65356E-08	1.19688E-07	3.93840E-02
1164	CO3(aq)	CO3(aq)	1.25799E-07	3.65269E-07	2.904	4.37894E-08	1.12625E-07	4.95659E-03
1165	NpO2-	NpO2-	9.49493E-06	1.88634E-08	1.987	3.30512E-09	8.50064E-09	2.28707E-03
1166	NpO2OH(aq)	NpO2OH(aq)	1.68316E-10	1.68316E-10	1.000	5.85892E-11	1.50689E-10	4.31052E-05
1167	H+	H+	8.66954E-11	3.39269E-10	3.913	1.01779E-11	7.76164E-11	7.82295E-08
1168	NpO2(OH)2-	NpO2(OH)2-	6.28105E-13	1.87627E-13	0.2987	2.18638E-13	5.62328E-13	1.70420E-07
1169	HCl(aq)	to titrate.acid.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.49E+02
1170	NaOH(aq)	to titrate.bases.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.94E+02
1171	NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-3.64E+08
1172	NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-3.05E+00
1173	Na3NpO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-9.31E+02
1174	NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-1.24E+01
1175	NaHCO3	NaHcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.29E+00
1176	Na2CO3.10H2O	Matron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-3.10E+00
1177	Na2CO3.7H2O	Na2CO3-Nephelinite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-3.14E+00
1178	Na2CO3.H2O	Thromhalite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.43E+00
1179	Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-4.70E+00
1180								
1181	pH (-log[ah+]); pmd(-log[md+])	9.4695	10.0620					
1182	Osmotic Coefficient=	1.241325						
1183	Equilibrium RH (%) =	77.812731						
1184	Ionic Strength (m) =	5.612017						
1185	Density, kg/m3	1188.81						
1186	fCO2(g); log[fCO2(g)] =			1.108E-05	-4.96			
1187								
1188	NOTES:							
1189	- Water "molality" is mole fraction H2O in aqueous phase							
1190	- Gas "molality" and "activity" are gas partial pressures							
1191	- "Descriptor" means:							
1192	*G/R/T=ln10 for species with nonzero concs. (convergence criterion)							
1193	*Saturation Index for minerals, SI=log10(IAP/Ksp)							
1194	*log10(activity) for aqueous species with very small concentrations							
1195	*log10(partial pressure) for gases							
1196								
1197	Total G/R=	-4.61721298E+03						
1198	Flashing Titration #	8						
1199	# inversions for batch pbm	29						
1200	benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.6molal NaCl							FMT V7.3
1201	DATABASE: HNS84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (HNS94);							
1202	95.01.31 Am(III)-Na-Cl-CO3-SO4-P04 (FMSR89, FMP90, P01, RFPF92, RFF94, RFF95)							
1203	Pressure= 1.00000E+00 [atm] Temperature= 3.98E+02 [-] Kelvin							
1204								
1205	Elemental Abundances for Flash Problem							
1206								
1207	Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter				
1208	3.86695692E+01	1.11018496E+02	9.93227291E+01	1.00177932E+05 Hydrogen				
1209	3.67172215E+01	5.55217779E+01	4.97075822E+01	7.95291491E+05 Oxygen				
1210	5.42967948E+00	5.61001045E+00	5.02253469E+00	1.15466917E+05 Sodium				
1211	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Potassium				
1212	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Magnesium				
1213	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Calcium				
1214	1.95138405E+00	5.60213091E+00	5.01565935E+00	1.77820171E+05 Chlorine				
1215	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Sulfur				
1216	3.47712639E+00	4.34048558E-03	3.88595344E-03	4.66741868E+01 Carbon				
1217	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 PosIon				
1218	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 NegIon				
1219	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Alf				
1220	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Boron				
1221	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Bromine				
1222	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 TracerEl				
1223	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Th(IV)				
1224	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Am(III)				
1225	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 U(VI)				
1226	3.47561578E+00	1.60501967E-06	1.22750493E-06	7.65074233E-01 Np(V)				
1227	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 ClO4-(EL)				
1228	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Phosphorus				
1229	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Electron				
1230	-1.20892820E-15	-3.47077543E-15	-3.10731863E-15	0.00000000E+00 Charge				

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

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1355 Cl- 5.59866E+00 5.27463E+00 0.9421 1.95190E+00 5.01240E+00 1.77705E+05
1356 CO3= 5.06627E-03 1.15070E-04 2.5957E-02 1.76629E-03 4.53578E-02 2.72187E+02
1357 HCO3- 1.09867E-03 4.06385E-04 0.3699 3.83037E-04 9.83623E-04 6.00178E+01
1358 OH- 1.01865E-04 5.56263E-05 0.5441 2.55141E-05 9.11987E-05 1.55104E+00 -1.56E-10
1359 HPO2(CO3)3== HPO2(CO3)3== 3.29354E-06 2.65024E-15 8.0466E-10 1.14825E-06 2.94666E-06 1.32417E+00
1360 HPO2(CO3)2== HPO2(CO3)2== 3.23222E-06 6.41283E-11 2.6028E-05 1.12687E-06 2.89376E-06 8.08E-10
1361 HPO2(CO3) HPO2(CO3) 1.33806E-07 2.43238E-07 1.818 4.86498E-08 1.19795E-07 3.84192E-02
1362 CO2(aq) 5.53405E-08 1.60997E-07 2.904 1.92938E-08 4.95452E-08 2.18049E-02 -9.19E-09
1363 HPO2+ 7.43248E-08 7.45944E-09 1.982 1.31200E-09 2.26917E-09 9.06466E-04 -7.94E-10
1364 HPO2OH(aq) HPO2OH(aq) 1.59617E-10 1.59617E-10 1.000 5.56486E-11 1.42930E-10 4.08781E-05 4.13E-09
1365 H+ 3.62550E-11 1.41496E-10 3.903 1.26398E-11 3.24586E-11 3.27150E-08 -4.92E-09
1366 HPO2(OH)2- HPO2(OH)2- 1.42919E-12 4.26699E-13 0.2986 4.98268E-13 1.27953E-12 3.87777E-07 9.06E-09
1367 HCl(aq) .....to titrate, acid only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.49E+02
1368 HNO3(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
1369 HPO2OH(aq) HPO2OH(aq) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.67E+00
1370 HPO2OH(amor) HPO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.66E+00
1371 Na3HPO2(CO3)2(=) DISABLED DISABLED 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -9.31E-02
1372 NaCl Malite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.25E-01
1373 NaHCO3 Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.26E+00
1374 Na2CO3.10H2O Natron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.70E+00
1375 Na2CO3.7H2O Na2CO3-Hepahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.74E+00
1376 Na2CO3.H2O Thermonatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.03E-00
1377 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
1378
1379 pH (-log[OH-]); pOH(-log[H+]) 9.8493 10.4406
1380 Osmotic Coefficient= 1.74893
1381 Equilibrium RH (%) = 77.824850
1382 Ionic Strength (m) = 5.615126
1383 Density, kg/m3 = 1188.79
1384 fCO2(g); log(fCO2(g))= 4.873E-06 -5.31
1385
1386 NOTES: - Water "molarity" is mole fraction H2O in aqueous phase
1387 Gas "molarity" and "activity" are gas partial pressures
1388 - "Descriptor" means:
1389 *O/R/T/In/O for species with nonzero concs. (convergence criteria)
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/R/E= -4.64072873E-03
1395 Flashing Titration # 10
1396 # inversions for batch pbm 28
1397
1398 BENCHMARK TITRATE Problem, LOG10 option; HPO(V)O2 with CO3 in 5.61molar NaCl FMT VI.3
1399 DATABASE: MHW84/PW88; HPO(V)-Na-CO3-OH-Cl-C1O4 (MHW84);
1400 95_01_31 Am(III)-Na-CO3-OH-Cl (FRM89, FR290, P91, RFF892, RFF94, RFF94)
1401 Pressure= 1.00000E+00 [atm] Temperature= 2.98E+02 [K] Kelvin
1402
1403 Elemental Abundances for Flash Problem
1404
1405 Total Moles Aq. Molarity Aq. Molarity Aq. mg/liter
1406 3.87560135E+01 1.11018651E+02 9.93943650E+01 1.00179480E+05 Hydrogen
1407 3.67651154E+01 5.55325555E+01 4.97203463E+01 7.95495709E+05 Oxygen
1408 5.43404174E+00 5.61002728E+00 5.02262026E+00 1.15468885E+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 1.95263769E+00 5.59343408E+00 5.00776448E+00 1.77540274E+05 Chlorine
1413 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1414 3.47868370E+00 8.0060113E-03 7.87911990E-03 9.4631031E+01 Carbon
1415 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1416 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Nitrogen
1417 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Aluminum
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 3.47868370E+00 1.2187218E+05 1.10901974E+05 2.6281114E+05 Np(V)
1425 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron
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 -1.61099060E-15 -4.61476789E-15 -4.13157112E-15 0.00000000E+00 Charge
1429
1430 Solution Parameters, Calculated
1431 SOLUTION MASS 463.521138924444 grams
1432 H2O MASS 349.094609954678 grams
1433 TDS (g/kg) 327.812362913951 g/kgH2O
1434
1435 Specified Solution Density 1188.78161259327 kg/m^3 = g/l
1436 DENSITY
1437
1438 Solution Parameters Based on Specified Density
1439 SOLUTION VOL 0.389922029424118 liters
1440 TDS 293.488236965686 g/l
1441
1442 Density based on TDS and NaCl solutions 1188.78161259327 g/l
1443 Percent relative error vs NaCl density 0.00000000000000E+000 %
1444
1445
1446
1447
1448 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1449
1450 Species Name Molarity Activity Act Coef Total Moles Molarity mg/liter Descriptor
1451 H2O WATER 8.31951E-01 7.78350E-01 0.9356 1.93770E+01 4.96966E+01 8.95293E+05
1452 Na3HPO2(CO3)2(=) Na3HPO2(CO3)2(=) 9.95607E+00 1.00000E+00 1.000 3.47561E+00 8.91361E+00 1.13800E+06
1453 H+ H+ 5.61003E+00 5.28539E+00 0.9421 1.95843E+00 5.02262E+00 1.15469E+05
1454 Cl- Cl- 5.59343E+00 5.28704E+00 0.9416 1.95264E+00 5.00776E+00 1.77540E+05
1455 CO3= CO3= 7.62562E-03 1.97880E-04 2.5949E-02 2.66206E-03 6.82717E-03 4.09693E+02
1456 HCO3- HCO3- 1.14291E-03 4.52533E-04 0.5441 3.98993E-04 1.02324E-03 4.24350E+01
1457 OH- OH- 1.47379E-04 8.02242E-05 0.5443 5.14493E-05 1.31948E-04 2.24408E+00 -2.20E-08
1458 HPO2(CO3)3== HPO2(CO3)3== 7.39875E-06 6.00222E-15 8.1125E-10 2.58268E-06 6.62405E-06 2.97469E+00 3.3E-08
1459 HPO2(CO3)2== HPO2(CO3)2== 4.85191E-06 1.26624E-10 2.6098E-05 1.69378E-08 4.34388E-08 1.69005E+00 1.76E-08
1460 HPO2(CO3) HPO2(CO3) 1.33905E-07 2.43306E-07 1.817 4.87454E-08 1.19848E-07 3.84488E-02 -7.9E-07
1461 CO2(aq) CO2(aq) 3.77510E-08 1.5435E-07 2.904 1.38768E-08 3.58888E-08 1.56626E-03 -2.9E-07
1462 HPO2+ HPO2+ 2.50641E-09 4.95882E-09 1.978 8.74975E-10 2.24398E-09 4.03735E-04 -1.77E-08
1463 HPO2OH(aq) HPO2OH(aq) 1.53583E-10 1.53583E-10 1.000 5.36149E-11 1.37502E-10 3.9329E-05 1.09E-07
1464 H+ H+ 2.51081E-11 9.77709E-11 3.894 8.76512E-12 2.24792E-11 2.26567E-08 -1.27E-07
1465 HPO2(OH)2- HPO2(OH)2- 1.42919E-12 5.94256E-13 0.2986 6.95155E-13 1.78281E-12 5.40300E-07 2.36E-07
1466 HCl(aq) .....to titrate, acid only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.49E+02
1467 HNO3(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
1468 HPO2OH(aq) HPO2OH(aq) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.09E+00
1469 HPO2OH(amor) HPO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.66E+00
1470 Na3HPO2(CO3)2(=) DISABLED DISABLED 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -9.31E-02
1471 NaCl Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.26E-01
1472 NaHCO3 Malite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.26E+00
1473 Na2CO3.10H2O Natron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.70E+00
1474 Na2CO3.7H2O Na2CO3-Hepahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.56E+00
1475 Na2CO3.H2O Thermonatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.85E+00
1476 Na3H(CO3)2.2H2O Trona 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -4.08E+00
1477
1478 pH (-log[OH-]); pOH(-log[H+]) 10.0098 10.6003

```


Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
1479 Osmotic Coefficient= 1.240532
1480 Equilibrium RH (%) = 77.834958
1481 Ionic Strength (m) = 5.617741
1482 Density, kg/m3 = 1188.78
1483 fCO2(g); log{fCO2(g)}= 3.501E-06 -5.46
1484
1485 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1486 - Gas "molality" and "activity" are gas partial pressures
1487 - "Descriptor" means:
1488 *G/RT/ln10 for species with nonzero concs. (convergence criterion)
1489 *saturation index for minerals, SI=log10(IAP/Ksp)
1490 *log10(activity) for aqueous species with very small concentrations
1491 *log10(partial pressure) for gases
1492
1493 Total G/RT= -4.64367246E+03
1494 Flashing Titration # 11
1495 # inversions for batch pblm 28
1496 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
1497 DATABASE: HSW64/FWS6; Np(V)-Na-CO3-OH-Cl-ClO4 (RSP4);
1498 95.01.31 Am(III)-Na-Cl-CO3-EO4-PO4 (FRSR89,FRF90,P91,RFR92,RFP94,RRFP94)
1499 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1500
1501 Elemental Abundances for Flash Problem
1502
1503 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
1504
1505 3.88284068E+01 1.11018771E+02 9.53954996E+01 1.00180724E+05 Hydrogen
1506 3.68052248E+01 5.55465070E+01 4.97309848E+01 7.9565918E+05 Oxygen
1507 5.43769997E+00 5.61004415E+00 5.02269243E+00 1.15470544E+05 Sodium
1508 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1509 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
1510 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
1511 1.95368755E+00 5.58601315E+00 5.00117739E+00 1.77306742E+05 Chlorine
1512 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1513 3.47998788E+00 1.25239828E-02 1.12127662E-02 1.34676535E+02 Carbon
1514 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 PosIon
1515 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 NegIon
1516 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Al3+
1517 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron
1518 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bismuth
1519 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 TracerEl
1520 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Th(IV)
1521 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Am(III)
1522 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 U(VI)
1523 3.47561578E+00 2.32128943E-05 2.07825866E-05 3.92647475E+00 Np(V)
1524 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 ClO4-(EL)
1525 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1526 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Electron
1527 -1.72202137E-15 -4.92362968E-15 -4.4081412E-15 0.00000000E+00 Charge
1528
1529 Solution Parameters, Calculated
1530 SOLUTION MASS 464.38515021376 grams
1531 H2O MASS 349.746321818895 grams
1532 TDS (g/kg) 127.777080834728 g/kgH2O
1533
1534 Specified Solution Density
1535 DENSITY 1188.76353136245 kg/m3 = g/l
1536
1537 Solution Parameters Based on Specified Density
1538 SOLUTION VOL 0.390645521977900 liters
1539 TDS 293.459983409118 g/l
1540
1541 Density based on TDS and NaCl solutions 1188.76353136245 g/l
1542 Percent relative error vs NaCl density 0.000000000000000E+000 %
1543
1544
1545 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1546
1547 Species Name Molality Activity Act Coef Total Moles Molarity mg/liter Descriptor
1548
1549 H2O WATER 8.31997E-01 7.78693E-01 0.9357 1.94140E+01 4.96971E+01 8.95304E+05
1550 NaHPO2CO3(s) NaHPO2CO3(s) 9.93751E+00 1.00000E+00 1.0000 3.47561E+00 8.89709E+00 1.13218E+06
1551 Na+ Na+ 5.61004E+00 5.28333E+00 0.9418 1.96209E+00 5.02269E+00 1.15471E+05
1552 Cl- Cl- 5.58601E+00 5.25591E+00 0.9409 1.95369E+00 5.00118E+00 1.77307E+05
1553 CO3- CO3- 1.12609E-02 2.92079E-04 2.5937E-02 1.93846E-03 1.00819E-02 6.05098E-02
1554 HCO3- HCO3- 1.20002E-03 4.43607E-04 0.3694 4.19981E-04 1.07510E-03 6.55992E-01
1555 OH- OH- 2.07122E-04 1.12810E-04 0.5447 7.24404E-05 1.85438E-04 3.15380E-09
1556 NpO2(CO3)1= NpO2(CO3)1= 1.59398E-05 1.38021E-14 8.2072E-10 5.57490E-06 1.42710E-05 6.40874E+00
1557 NpO2(CO3)2= NpO2(CO3)2= 7.13717E-06 1.86975E-10 2.6197E-05 2.49620E-06 6.38993E-06 2.48610E+00
1558 NpO2CO3- NpO2CO3- 1.34044E-07 2.43401E-07 1.816 4.68815E-08 1.20010E-07 3.94902E-02
1559 CO2(aq) CO2(aq) 2.95765E-08 6.61855E-08 2.904 1.03792E-08 2.65695E-08 1.16932E-03
1560 NpO2+ NpO2+ 1.70329E-09 3.36086E-09 1.973 5.95718E-10 1.52496E-09 4.10285E-04
1561 NpO2OH(aq) NpO2OH(aq) 1.46370E-10 1.46370E-10 1.000 5.11925E-11 1.31046E-10 3.74863E-05
1562 H+ H+ 1.79163E-11 6.95424E-11 3.882 6.26615E-12 1.60405E-11 1.61672E-08
1563 NpO2(OH)2- NpO2(OH)2- 2.67040E-12 7.96388E-13 0.2962 9.33963E-13 2.39062E-12 7.24565E-07
1564 HCl(aq) .....to.titrate.acid.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1565 NaOH(aq) .....to.titrate.base.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1566 NpO2OH(aged) NpO2OH(aged) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1567 NpO2OH(amor) NpO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1568 Na3NpO2(CO3)2(s)_DISABLED_DISABLED 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1569 NaCl Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1570 NaHCO3 NaHCO3 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1571 Na2CO3.10H2O Na2CO3.10H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1572 Na2CO3.7H2O Na2CO3.7H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1573 Na2CO3.H2O Na2CO3.H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1574 Na3H(CO3)2.2H2O Na3H(CO3)2.2H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1575
1576 pH (-log{aH+}); pOH(-log{aOH-}) 10.1578 10.7468
1577 Osmotic Coefficient= 1.240021
1578 Equilibrium RH (%) = 77.849336
1579 Ionic Strength (m) = 5.621486
1580 Density, kg/m3 = 1188.76
1581 fCO2(g); log{fCO2(g)}= 2.614E-06 -5.58
1582
1583 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1584 - Gas "molality" and "activity" are gas partial pressures
1585 - "Descriptor" means:
1586 *G/RT/ln10 for species with nonzero concs. (convergence criterion)
1587 *saturation index for minerals, SI=log10(IAP/Ksp)
1588 *log10(activity) for aqueous species with very small concentrations
1589 *log10(partial pressure) for gases
1590
1591 Total G/RT= -4.64786705E+03
1592 Flashing Titration # 12
1593 # inversions for batch pblm 28
1594 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
1595 DATABASE: HSW64/FWS6; Np(V)-Na-CO3-OH-Cl-ClO4 (RSP4);
1596 95.01.31 Am(III)-Na-Cl-CO3-EO4-PO4 (FRSR89,FRF90,P91,RFR92,RFP94,RRFP94)
1597 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1598
1599 Elemental Abundances for Flash Problem
1600
1601 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
1602
```

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

1603	3.89315747E+01	1.11018923E+02	9.93971848E+01	1.00182423E+05	Hydrogen
1604	3.68623846E+01	5.55624877E+01	4.97460679E+01	7.95907238E+05	Oxygen
1605	5.44291331E+00	5.61007250E+00	5.62279611E+00	1.15472927E+05	Sodium
1606	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
1607	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
1608	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1609	1.95518172E+00	5.57548444E+00	4.99182884E+00	1.76975108E+05	Chlorine
1610	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
1611	3.48184547E+00	1.78114648E-02	1.59469162E-02	1.91538411E+02	Carbon
1612	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Positron
1613	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neutron
1614	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Air
1615	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
1616	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
1617	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerE
1618	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Tb(IV)
1619	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
1620	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
1621	3.47561578E+00	4.37699198E+00	3.91872342E+00	5.28262133E+00	Hp(V)
1622	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4-(EL)
1623	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
1624	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
1625	-1.77023110E-15	-5.04806576E-15	-4.51962164E-15	0.00000000E+00	Charge

1626
1627
1628 Solution Parameters, Calculated
1629 SOLUTION MASS 465.601420606259 grams
1630 H2O MASS 350.675126352089 grams
1631 TDS (g/kg) 327.728674256698 g/kgH2O
1632
1633 Specified Solution Density
1634 DENSITY 1188.73872346794 kg/m³ = g/l
1635
1636 Solution Parameters Based on Specified Density
1637 SOLUTION VOL 0.391676034795075 liters
1638 TDS 293.421218812867 g/l
1639
1640 Density based on TDS and NaCl solutions 1188.73872346794 g/l
1641 Percent relative error vs NaCl density 0.000000000000E+000 %
1642
1643
1644
1645

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.32061E-01	7.78597E-01	0.9359	1.94655E+01	4.96979E+01	8.95318E+05	
NaHPO2CO3(a)	9.91117E+00	1.00000E+00	1.000	2.47560E+00	8.07364E+00	3.12393E+06	
Na+	5.61007E+00	5.28057E+00	0.9413	1.96731E+00	5.02280E+00	1.5473E+05	
Cl-	5.57548E+00	5.24002E+00	0.9398	1.95518E+00	4.99183E+00	1.76975E+05	
CO3=	1.64154E-02	4.25480E-04	2.5920E-02	5.75848E-03	1.46970E-02	8.61956E-02	
NaCO3-	1.27533E-03	4.70618E-04	0.3690	4.67327E-04	1.14183E-03	6.96709E-01	
OH-	2.84255E-04	1.54942E-04	0.5451	9.96812E-05	2.54499E-04	4.32633E+00	-1.39E-03
NpO2(CO3)3=	3.32873E-05	2.77756E-14	8.3442E-10	1.16730E-05	2.98027E-05	1.33636E+01	5.09E-03
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-	1.34242E-07	2.43528E-07	1.814	4.70755E-08	1.20190E-07	9.95491E-02	6.17E-12
CO2(aq)	2.29199E-08	6.65707E-08	2.904	8.03744E-09	2.05206E-08	9.01078E-04	-7.33E-08
NpO2	1.17423E-09	2.30833E-09	1.966	4.11805E-10	1.05133E-09	2.82874E-04	-2.44E-09
NpO2OH(aq)	1.38078E-10	1.38078E-10	1.000	4.84205E-11	1.23624E-10	2.53631E-05	3.36E-08
H+	1.31074E-11	5.06455E-11	3.864	4.59643E-12	1.17532E-11	1.18280E-08	-3.61E-08
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)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.56E+02
NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.94E+02
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.13E+00
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.73E+00
NaHPO2(CO3)2(a) DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.30E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.28E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.20E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.23E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.52E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.70E+00

1676 pH (-log(aH+)); pOH(-log(aOH+)) 10.2955 10.0825
1677 Osmotic Coefficient= 1.239297
1678 Equilibrium pH (s) = 77.869707
1679 Ionic strength (m) = 5.626852
1680 Density, kg/m3 = 1188.74
1681 fCO2(g); log(fCO2(g))= 2.019E-06 -5.69

1682
1683 NOTES: - Water 'molality' is mole fraction H2O in aqueous phase
1684 Gas 'molality' and 'activity' are gas partial pressures
1685 - 'Descriptor' means:
1686 *DG/RT/ln10 for species with nonzero concs. (convergence criterion)
1687 *Saturation Index for minerals, SI=log10(IAP/Ksp)
1688 *log10(activity) for aqueous species with very small concentrations
1689 *log10(partial pressure) for gases

1690
1691 Total O/RT= -4.65384406E+03
1692 Flashing Titration # 13
1693 # inversions for batch pbm 28
1694 Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.1
1695 DATABASE: IGM84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (HR94)
1696 95.01.31 Am(III)-Na-Cl-CO3-SO4-Pb4 (FRLSR8), RFX90.991, RFR92, RFP94, RUP94
1697 Pressure= 1.00000E+00 [atm] Temperature= 2.98E+02 [K] Kelvin
1698
1699

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.89785996E+01	1.11019115E+02	9.93994493E+01	1.00184705E+05	Hydrogen
3.69438403E+01	5.55815308E+01	4.97674088E+01	7.96248680E+05	Oxygen
5.45034287E+00	5.6102129E+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
1.9571591E+00	5.56057488E+00	4.97858483E+00	1.76505768E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.48449515E+00	2.53082323E-02	2.26593804E-02	2.72161818E+02	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Positron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neutron
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	TracerE
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	4.36520364E-05	7.4010326E-05	1.75440146E-01	Hp(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	-4.48603272E-15	-4.19557544E-15	0.00000000E+00	Charge

Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
1727 Solution Parameters, Calculated
1728 SOLUTION MASS 467.335943430018 grams
1729 H2O MASS 351.998839687452 grams
1730 TDS(g/kg) 327.663306631852 g/kgH2O
1731
1732 Specified Solution Density
1733 DENSITY 1188.70522197651 kg/m3 = g/l
1734
1735 Solution Parameters Based on Specified Density
1736 SOLUTION VOL 0.393147043346002 liters
1737 TDS 293.368869726077 g/l
1738
1739 Density based on TDS and NaCl solutions 1188.70522197651 g/l
1740 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	8.32153E-01	7.78885E-01	0.9361	1.95390E+01	4.96889E+01	8.95336E+05	
NaHPO2CO3(s)	NaHPO2CO3(s)	1.00000E+00	1.0000	3.47559E+00	8.84042E+00	3.11224E+06	
Na+	5.61012E+00	5.27693E+00	0.9406	1.97476E+00	5.02295E+00	1.15476E+05	
Cl-	5.56057E+00	5.21732E+00	0.9383	1.95732E+00	4.97858E+00	1.76506E+05	
CO3-	2.37058E-02	6.13801E-04	2.5892E-02	8.34440E-03	2.12246E-02	1.27367E+03	
HCO3-	1.36956E-03	5.04583E-04	0.3684	4.82083E-04	1.22622E-03	7.48201E+01	
OH-	3.82200E-04	2.08552E-04	0.5457	1.34534E-04	3.42198E-04	5.81986E+00	-1.15E-09
NpO2(CO3)3---	NpO2(CO3)3---	6.77047E-05	5.78442E-14	8.5436E-10	2.38320E-05	6.06184E-05	3.43E-09
NpO2(CO3)2--	NpO2(CO3)2--	1.48219E-05	3.93404E-10	2.6542E-05	5.21729E-06	1.32706E-05	5.16313E+00
NpO2CO3-	NpO2CO3-	1.34522E-07	2.43696E-07	1.812	4.73516E-08	1.20442E-07	3.96323E-02
CO2(aq)	CO2(aq)	1.82542E-08	5.30275E-08	2.905	6.42544E-09	1.63436E-08	-6.76E-08
NpO2+	NpO2+	8.18986E-10	1.60121E-09	1.955	2.88282E-10	7.33267E-10	-1.63E-09
NpO2OH(aq)	NpO2OH(aq)	1.28920E-10	1.28920E-10	1.000	4.53797E-11	1.15427E-10	3.13E-08
H+	H+	9.80463E-12	3.74405E-11	3.839	3.45122E-12	8.77445E-12	-3.29E-08
NpO2(OH)2-	NpO2(OH)2-	4.35857E-12	1.29678E-12	0.2975	1.53419E-12	3.90234E-12	1.18265E-04
HCl(aq).....to.titrates.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.50E+02
NaOH(aq).....to.titrates.base.only		0.00000E+00	0.00000E+00	1.000	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	-3.16E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-3.76E+00
NaH2PO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-9.30E+02
NaCl	NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-1.31E-01
NaHCO3	NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.17E+00
Na2CO3.10H2O	Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.03E+00
Na2CO3.7H2O	Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.07E+00
Na2CO3.H2O	Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.36E+00
NaH(CO3)2.2H2O	NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-3.51E+00

```
1744 pH (-log[act+]); pM(-log[m+]) 10.4243 11.0086
1745 Osmotic Coefficient= 1.238276
1746 Equilibrium RM (%) = 77.898521
1747 Ionic Strength (m) = 5.634549
1748 Density, kg/m3 = 1188.71
1749 fCO2(g); log(fCO2(g)) = 1.608E-06 -5.79
1750
1751 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1752 - Gas "molality" and "activity" are gas partial pressures
1753 - "Descriptor" means:
1754 *OG/RT/ln10 for species with nonzero charges. (convergence criterion)
1755 *Saturation Index for minerals. SI=log10(IAP/Ksp)
1756 *log10(activity) for aqueous species with very small concentrations
1757 *log10(partial pressure) for gases
```

```
1758 Total O/RT= -4.66216092E-03
1759 Flashing Titration # 14
1760 # Inversions for batch phin 38
1761 Benchmark TITRATE Problem. LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl PHR V2.3
1762 DATABASE: IOW64/PW66; Np(V)-Na-CO3-OH-Cl-C104 (NR94);
1763 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (PRR89, PRF90, P91, RFF92, RFF94, RUFF94)
1764 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	5.61020535E+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
1.96035402E+00	5.53951836E+00	4.95987023E+00	1.75842279E+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	Phosphorus
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	Neptunium
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	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

```
1826 Solution Parameters, Calculated
1827 SOLUTION MASS 469.810029265022 grams
1828 H2O MASS 353.885368468190 grams
1829 TDS(g/kg) 327.576868460591 g/kgH2O
1830
1831 Specified Solution Density
1832 DENSITY 1188.66091947607 kg/m3 = g/l
1833
1834 Solution Parameters Based on Specified Density
1835 SOLUTION VOL 0.39524310211397 liters
1836 TDS 293.239843065870 g/l
1837
1838 Density based on TDS and NaCl solutions 1188.66091947607 g/l
1839 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	8.32282E-01	7.79391E-01	0.9365	1.96437E+01	4.97003E+01	8.95361E+05	
NaHPO2CO3(s)	NaHPO2CO3(s)	1.00000E+00	1.0000	3.47556E+00	8.79348E+00	3.09571E+06	
Na+	5.61021E+00	5.27303E+00	0.9398	1.98537E+00	5.02316E+00	1.15481E+05	
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"

```

1851 CO3= CO3= 3.39812E-02 8.78458E-04 2.5851E-02 1.20255E-02 3.04255E-02 1.82581E-03
1852 HCO3= HCO3= 1.48672E-01 5.46468E-04 0.3676 5.26128E-04 1.33115E-03 8.12230E-01
1853 OH= OH= 5.04519E-04 2.5741E-04 0.5444 1.78577E-04 4.51816E-04 7.68417E+00 -1.19E-09
1854 HPO2(CO3)3== HPO2(CO3)3== 1.34208E-04 1.18584E-13 8.8359E-10 4.74943E-05 1.20165E-04 5.39629E+01 2.60E-09
1855 HPO2(CO3)2== HPO2(CO3)2== 2.10028E-05 5.83525E-10 2.4831E-05 7.43240E-06 1.86051E-05 7.11643E+00 1.17E-09
1856 HPO2CO3= HPO2CO3= 1.34816E-07 2.43910E-07 1.808 4.77447E-08 1.20798E-07 3.97498E-02 5.27E-12
1857 CO2(aq) CO2(aq) 1.49488E-08 4.34356E-08 2.906 5.25018E-09 1.33845E-08 5.89054E-04 -7.10E-08
1858 HPO2= HPO2= 5.77122E-10 1.11579E-09 1.940 2.04235E-10 5.16732E-10 1.39025E-04 -1.24E-09
1859 HPO2OH(aq) HPO2OH(aq) 1.19205E-10 1.19205E-10 1.000 4.21850E-11 1.06732E-10 3.05311E-05 3.24E-08
1860 H+ H+ 7.48731E-12 2.84636E-11 3.804 2.64966E-12 6.70386E-12 6.75682E-09 -3.36E-08
1861 HPO2(OH)2= HPO2(OH)2= 5.33952E-12 1.58534E-12 0.2969 1.88958E-12 4.78080E-12 1.44888E-06 6.60E-08
1862 HCl(aq).....to.titrata.acid.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.50E-02
1863 NaOH(aq).....to.titrata.base.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.93E-02
1864 HPO2OH(aq) HPO2OH(aq) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.30E-02
1865 HPO2OH(amor) HPO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.79E-02
1866 Na3HPO2(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
1867 NaCl Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.34E-01
1868 NaHCO3 NaHCO3 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.14E-01
1869 Na2CO3.10H2O Natron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.87E-01
1870 Na2CO3.7H2O Na2CO3-Heptahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.91E-01
1871 Na2CO3.H2O Thermonatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.20E-01
1872 Na3H(CO3)2.2H2O Trona 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.32E-01
1873
1874 pH (-log(aH+)); pOH(-log(aOH)) 10.5454 11.1257
1875 Osmotic Coefficient= 1.234838
1876 Equilibrium RH (%) = 77.93147
1877 Ionic Strength (m) = 5.645593
1878 Density, kg/m3 = 1188.66
1879 fCO2(g); log(fCO2(g)) 1.317E-06 -5.88
1880
1881 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1882 - Gas "molality" and "activity" are gas partial pressures
1883 - "Descriptor" means:
1884 "dg/RT/ln10 for species with nonzero concs. (convergence criterion)
1885 "saturation index for minerals, SI=log10(IAP/Ksp)
1886 "log10(activity) for aqueous species with very small concentrations
1887 "log10(partial pressure) for gases
1888
1889 Total G/RT= -4.67449693E+03
1890 Flashing Titration # 15
1891 # Inversions for batch pbm 20
1892 Benchmark: TITRATE Problem, LOG10 option; H2O(V)2 with CO2 in 5.61molal NaCl FMT V2.3
1893 DATABASE: HSW4/FM8, H2O(V)-Na-CO3-OH-Cl-ClO4 (HSW4)
1894 95.01.31 Am(III)-Na-Cl-CO3-SO4-P94 (FRSR8,FRP90,FR1,FRFR2,FRFR4,FRFR94)
1895 Pressure= 1.00000E+00 [a] ATM Temperature= 2.98E+02 [a] Kelvin
1896
1897 Elemental Abundances for Flash Problem
1898
1899 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
1900
1901 3.95867206E+01 1.11019649E+02 3.94062599E+01 1.00191569E+05 Hydrogen
1902 3.72253652E+01 5.56424986E+01 4.98398335E+01 7.97407433E+05 Oxygen
1903 5.47601956E+00 5.61035435E+00 5.02347422E+00 1.15488517E+05 Sodium
1904 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1905 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
1906 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
1907 1.96468480E+00 5.50989354E+00 4.93352277E+00 1.74908165E+05 Chlorine
1908 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1909 3.49364905E+00 5.08618173E-02 4.55413352E-02 5.46996977E+02 Carbon
1910 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Selenium
1911 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Arsenic
1912 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Alr
1913 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron
1914 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bromine
1915 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 TracerEl
1916 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Th(IV)
1917 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Am(III)
1918 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 U(VI)
1919 3.47561578E+00 2.88102498E-04 2.57965074E-04 6.11501564E+01 Np(V)
1920 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 ClO4-(EL)
1921 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1922 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Electron
1923 -1.36636579E-15 -3.83192766E-15 -3.43108272E-15 0.00000000E+00 Charge
1924
1925 Solution Parameters, Calculated
1926 SOLUTION MASS 473.339684533624 grams
1927 H2O MASS 356.574003417585 grams
1928 TDS(g/kg) 327.465491925420 g/kgH2O
1929
1930 Specified Solution Density
1931 DENSITY 1188.6038311845 kg/m3 = g/l
1932
1933 Solution Parameters Based on Specified Density
1934 SOLUTION VOL 0.398331646549673 liters
1935 TDS 293.210437350988 g/l
1936
1937 Density based on TDS and NaCl solutions 1188.6038311845 g/l
1938 Percent relative error vs NaCl density 0.000000000000000E+000 %
1939
1940
1941
1942 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1943
1944 Species Name Molality Activity Act Coef Total Moles Molarity mg/liter Descriptor
1945
1946 H2O WATER 8.32465E-01 7.79962E-01 0.9369 1.97930E+01 4.97021E-01 8.95393E+05
1947 Na3HPO2CO3(s) Na3HPO2CO3(s) 9.74696E-01 1.00000E+00 1.000 3.47551E+00 8.72736E-01 3.07243E+04
1948 Na+ Na+ 5.61035E+00 5.26665E+00 0.9387 2.00051E+00 5.02347E+00 1.15489E+05
1949 Cl- Cl- 5.50989E+00 5.13884E+00 0.9327 1.96468E+00 4.93352E+00 1.74908E+05
1950 CO3= CO3= 4.81971E-02 1.24807E-03 2.5788E-02 1.72571E-02 4.33344E-02 2.60046E+01
1951 HCO3= HCO3= 1.63010E-03 5.97142E-04 0.3663 5.81251E-04 1.45959E-03 8.90593E+01
1952 OH= OH= 5.55397E-04 1.56792E-04 0.5474 2.33698E-04 5.86839E-04 9.98054E+00
1953 HPO2(CO3)3== HPO2(CO3)3== 2.58546E-04 2.39623E-13 5.2681E-10 9.21906E-05 2.31500E-04 1.03981E+02 2.16E-09
1954 HPO2(CO3)2== HPO2(CO3)2== 2.94209E-05 8.01487E-10 2.7424E-05 1.04907E-05 2.63433E-05 1.02493E+01 5.99E-10
1955 HPO2CO3= HPO2CO3= 1.35468E-07 2.44172E-07 1.802 4.83043E-08 1.21297E-07 3.99135E-02 6.05E-12
1956 CO2(aq) CO2(aq) 1.25492E-08 3.64751E-08 2.907 4.47472E-09 1.12365E-08 4.94515E-04 -8.59E-08
1957 HPO2= HPO2= 4.11022E-10 7.89015E-10 1.930 1.48560E-10 2.68027E-10 9.90165E-05 -1.06E-09
1958 HPO2OH(aq) HPO2OH(aq) 1.99291E-10 1.09291E-10 1.000 3.89705E-11 9.78589E-11 2.79929E-05 1.64E-08
1959 HPO2(OH)2= HPO2(OH)2= 6.38945E-12 1.89128E-12 0.2960 2.28313E-12 5.72107E-12 1.73384E-06 7.43E-08
1960 H+ H+ 5.83272E-12 2.19064E-11 3.756 2.07980E-12 5.22258E-12 5.26384E-09 -3.76E-08
1961 HCl(aq).....to.titrata.acid.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.50E+02
1962 HNO3(aq).....to.titrata.base.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.93E+02
1963 HPO2OH(amor) HPO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.23E+00
1964 HPO2OH(aq) HPO2OH(aq) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.83E+00
1965 Na3HPO2(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
1966 NaCl Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.38E-01
1967 NaHCO3 NaHCO3 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.10E+00
1968 Na2CO3.10H2O Natron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.72E+00
1969 Na2CO3.7H2O Na2CO3-Heptahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.76E+00
1970 Na2CO3.H2O Thermonatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.05E+00
1971 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
1972
1973 pH (-log(aH+)); pOH(-log(aOH)) 10.5594 11.2341
1974 Osmotic Coefficient= 1.234833

```


Appendix M: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
1975 Equilibrium RH (%) = 77.996177
1976 Ionic strength (m) = 5.651425
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+01
1989 TITRATE file name is U1:[SCRABD.FMT.UN]NP_NACL_BM_LOG.TITRATE:1
```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

See Table 15 for explanation of this listing.

```

1 INPUT file name is:U1:(SCRABP.FMT.UN)NP_NACL_BM_LIN.IN;1
2 INGRESS file name is:U1:(SCRABP.FMT.UN)NP_NACL_BM_LIN.INGRESS;1
3 OUTPUT file name is:U1:(SCRABP.FMT.UN)NP_NACL_BM_LIN.OUT;1
4 CHEMSTAT file name is U1:(SCRABP.FMT.UN)FMT_NSM_NP_AM_RTEST.CHEMSTAT;1
5 Temperature is Hard Coded as 298.15K
6 Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molar NaCl FMT V2.3
7 DATABASE: HW84/PW86; Np(V)-Na-CO3-OH-Cl-C104 (HW84);
8 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,TRF90,P91,APFR92,RFF94,RUFF94)
9
10 Accuracy of reactions is 1.0000E-06
11 Minimum elemental abundance is 1.0000E-18
12 Number of Aqueous Species is 50
13
14 PITZER Data Base NOT Echoed in this Run
15
16 Species Order for Pitzer Parameters
17
18 Cations 13
19
20 Na+      K+      Ca++     Mg++     MgOH+    H+
21 MgB(OH)4+ CaB(OH)4+ Am+++    AmCO3+   Th+++    UO2++
22 NpO2+
23
24 Anions 20
25 Cl-      SO4=     HSO4-    OH-      HCO3-    CO3=
26 B(OH)4-  B(OH)4-  B(OH)4-  Br-      Am(CO3)2- Am(CO3)3+-
27 ClO4-    pe NpO2(OH)2- NpO2CO3- NpO2(CO3)2-- NpO2(CO3)3--- H2PO4-
28 HPO4=
29
30 Neutral 6
31 CO2(aq)  CaCO3(aq) MgCO3(aq) B(OH)3(aq) NpO2OH(aq) H3PO4(aq)
32
33 using PITZER ACTIVITY COEFFICIENT model
34 Charge Balance replaces element Oxygen
35
36 this is a TITRATION problem
37
38 Ideal Gas Constant is Unity (Dimensionless)
39 Temperature = 298.15 [=] Degree Kelvin
40
41
42
43
44
45
46
47 115 Species      23 Elements
48
49 Element Name      Molecular Weight
50 Hydrogen           1.00790
51 Oxygen            15.99940
52 Sodium            22.98977
53 Potassium         39.09830
54 Magnesium         24.30500
55 Calcium           40.08000
56 Chlorine          35.45300
57 Sulfur            32.06000
58 Carbon            12.01100
59 Phosphorus        30.97400
60 Nitrogen          14.00640
61 Air               28.84000
62 Boron             10.81000
63 Bromine           79.90400
64 TracerEl         0.00000
65 Th(Iv)            232.03810
66 Am(III)           243.00000
67 U(VI)             238.02900
68 Np(V)             237.04820
69 ClO4- (EL)       99.45060
70 Phosphorus       30.97400
71 Electron         0.00000
72 Charge           0.00000
73
74
75
76 Species Name      Phase      Mol.Wt.      Std Chemical Potential, u/RT
77 1 H2O              aqueous    18.015        -95.6635
78 2 Na+              aqueous    22.990        -105.6510
79 3 K+               aqueous    39.098        -113.9570
80 4 Ca++             aqueous    40.080        -223.3000
81 5 Mg++             aqueous    24.305        -183.4680
82 6 MgOH+            aqueous    41.312        -251.9400
83 7 H+               aqueous    1.008         0.0000
84 8 Cl-              aqueous    35.453        -52.9550
85 9 SO4=             aqueous    96.058        -302.3860
86 10 HSO4-           aqueous    97.066        -304.9420
87 11 OH-             aqueous    17.007        -63.4350
88 12 HCO3-           aqueous    61.017        -236.7510
89 13 CO3=            aqueous    60.009        -212.9480
90 14 CO2(aq)         aqueous    44.010        -155.6800
91 15 CaCO3(aq)       aqueous    100.089       -443.5000
92 16 MgCO3(aq)       aqueous    84.314        -403.1550
93 17 B(OH)3(aq)      aqueous    61.832        -390.8100
94 18 B(OH)4-         aqueous    78.839        -465.2000
95 19 B(OH)3(OH)4-    aqueous    148.457       -963.7700
96 20 B(OH)4(OH)4-    aqueous    191.266       -1239.1000
97 21 CaB(OH)4+       aqueous    118.919       -692.3000
98 22 MgB(OH)4+       aqueous    103.144       -651.8900
99 23 Br-              aqueous    79.904        -999.9900
100 24 ClO4-            perchlorate ClO4- aqueous    99.451       -999.9900
101 25 NaOH(aq)         to titrate base only aqueous    39.997       500.0000
102 26 HCl(aq)          to titrate acid only aqueous    36.461       500.0000
103 27 HClO4(aq)        to titrate acid only aqueous    100.459      500.0000
104 28 PosIon          POSITIVE ION aqueous    0.000        0.0000
105 29 NegIon          NEGATIVE ION aqueous    0.000        0.0000
106 30 PosIon(OH)(aq)  to titrate base aqueous    17.007       500.0000
107 31 NegIon(aq)       to titrate acid aqueous    1.008        500.0000
108 32 Tracer(aq)       conservative tracer aqueous    0.000        0.0000
109 33 H2PO4(aq)        H2PO4- aqueous    97.973       -499.2999
110 34 H2PO4-           H2PO4- aqueous    96.967       -455.9600
111 35 HPO4=            HPO4= aqueous    95.980       -439.1670
112 36 PO4=             PO4=-- aqueous    94.972       -410.9470
113 37 NpO2+            NpO2+ aqueous    269.047      -369.1270
114 38 NpO2OH(aq)      NpO2OH(aq) aqueous    285.054      -438.5180
115 39 NpO2(OH)2-      NpO2(OH)2- aqueous    303.062      -505.8290
  
```


Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

363 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	5.57464E-01	8.59843E-01	1.003	5.55025E+01	5.00446E-01	9.01564E+05	
Na+	5.61062E+00	3.69801E+00	0.6593	5.61000E+00	5.05833E+00	1.16290E+05	
CO3-	1.99407E+00	4.09214E-02	2.0522E-02	1.99385E+00	1.79778E+00	1.07884E+05	
Cl-	1.51038E+00	1.04677E+00	0.6613	1.51000E+00	1.45148E+00	5.14644E+04	
HCO3-	6.14734E-03	1.59048E-03	0.2517	6.14666E-03	5.54221E-03	3.38170E+02	
OH-	6.14733E-03	4.86901E-03	0.7921	6.14666E-03	5.54221E-03	9.42580E+01	2.07E-11
CO2(aq)	2.36875E-09	1.75913E-09	3.022	2.36850E-09	2.13559E-09	9.39686E-05	-2.10E-07
H+	2.39548E-12	1.77959E-12	0.7416	2.39527E-12	2.16334E-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	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.30E+02
Na2CO3.H2O	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.99E-01
Na2CO3.7H2O	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.51E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.83E+00
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.57E+00

384 pH (-log[M+]); pOH(-log[OH-]) 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

391 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
 392 - Gas "molality" and "activity" are gas partial pressures
 393 - "Descriptor" means:
 394 *G/R/T/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 Total G/R/T= -6.42133776E+03
 400 Reaction # 1 sidsum 2.00000000000000
 401 This is a solid-only reaction

402 shifting left by 4.64434654478256
 403 calling makemuv for allomorphic reactions
 404 # inversions for batch phin 99
 405 Benchmark TITRATE Problem, LINEAR option; Np(VIC2 with CO3 in 5.61molar NaCl PWT V2.3
 406 DATABASE: IHW84/PW86; Np(V)-Na-CO3-ON-Cl-C104 (HM84)
 407 95.01.31 Na(III)-Na-Cl-CO3-SO4-PO4 (PRFR89,FRP90,FR91,RRFP92,RRFP94,RRFP94)

408 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
 409
 410 Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1.11018363E+02	1.11017591E+02	9.9388868E+01	1.00169020E+05	Hydrogen
1.05508682E+02	5.55113597E+01	4.96942389E+01	7.95078006E+05	Oxygen
1.56100000E+01	5.61057382E+00	5.02263316E+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
5.61100000E+00	5.61096098E+00	5.02279775E+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	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Argon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neon
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

411
 412 Solution Parameters, Calculated
 413 SOLUTION MASS 1328.11614865108 grams
 414 H2O MASS 1000.00695466820 grams
 415 TDS (g/kg) 328.106912108174 g/kgH2O
 416
 417 Specified Solution Density 1188.93254605458 kg/m3 = g/l
 418 DENSITY
 419
 420 Solution Parameters Based on Specified Density
 421 SOLUTION VOL 1.11706602116190 liters
 422 TDS 293.724084133903 g/l
 423
 424 Density based on TDS and NaCl solutions 1188.93254605458 g/l
 425 Percent relative error vs NaCl density 0.00000000000000E+000 %

426 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31822E-01	7.77959E-01	0.9352	5.55091E+01	4.96918E+01	8.95208E+05	
NaHPO2CO3(a)	9.99932E+00	1.00000E+00	1.000	9.99939E+00	8.95147E+00	3.15133E+04	
Cl-	5.61096E+00	5.29232E+00	0.9434	5.61000E+00	5.02298E+00	1.78080E+05	
Na+	5.61057E+00	5.29268E+00	0.9433	5.61061E+00	5.02263E+00	1.15469E+05	
HPO2-	6.12705E-04	1.21978E-03	1.991	6.12709E-04	5.48499E-04	1.47572E+02	
CO2(aq)	3.86103E-04	1.12115E-03	2.904	3.86106E-04	3.45643E-04	1.52117E+01	
HCO3-	2.26571E-04	8.38810E-05	0.3702	2.26573E-04	2.02829E-04	1.23760E+01	1.23E-14
H+	1.21872E-06	4.78095E-06	3.922	1.21873E-06	1.09101E-06	1.09962E-03	1.23E-14
HPO2CO3-	1.33526E-07	9.87897E-07	1.820	1.33527E-07	1.19534E-07	3.93334E-02	1.85E-14
CO3-	3.09384E-08	8.03343E-10	2.5946E-02	3.09386E-08	2.76963E-08	1.46203E-03	0.00E+00
OH-	3.01485E-09	1.63977E-09	0.5435	3.01687E-09	2.70071E-09	4.59318E-05	1.23E-14
HPO2OH(aq)	7.72186E-10	7.72186E-10	1.000	7.72191E-10	6.91267E-10	1.97740E-04	-6.17E-15
HPO2(CO3)2-	1.98384E-11	5.13355E-16	2.5877E-05	1.98385E-11	1.77595E-11	6.90960E-06	0.00E+00
HPO2(OH)2-	2.04818E-16	6.10703E-17	0.2988	2.04819E-16	1.82964E-16	5.54494E-11	0.00E+00
HPO2(CO3)3--	1.25197E-16	9.87897E-26	7.8908E-10	1.25198E-16	1.12077E-16	5.03110E-11	-2.35E-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	-2.92E+02
HPO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+02
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.24E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.95E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.91E+00
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+00
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E+01
Na3HPO2(CO3)2(s)_DISABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.26E-02
HPO2OH(aqgd)	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"

487
488 pH (-log(aH+)); pOH(-log(mOH+)) 5.3205 5.9141
489 Osmotic Coefficient= 1.241871
490 Equilibrium RH (%) = 77.795863
491 Ionic Strength (m) = 5.611188
492 Density, kg/m3 = 1188.93
493 fCO2(g); log(fCO2(g))= 3.400E-02 -1.47
494
495 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
496 - Gas "molality" and "activity" are gas partial pressures
497 - "Descriptor" means:
498 *G/R/T/ln10 for species with nonzero concs. (convergence criterion)
499 *Saturation Index for minerals, SI=log10(IAP/Ksp)
500 *log10(activity) for aqueous species with very small concentrations
501 *log10(partial pressure) for gases
502
503 Total G/R/T= -1.33223084E+04
504 Flashing Titration # 1
505 # Inversions for batch pblm 17
506 Benchmark TITRATE Problem, LINEAR option: Np(V)O2 with CO2 in 5.61molal NaCl PWT V2.1
507 DATABASE: NWS4/FWS6; Np(V)-Na-CO3-OH-Cl-C1O4 (NR94)
508 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRFR89,FRF90,PP1,RPFR92,RPF94,RRFF94)
509 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
510
511 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	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Argon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Krypton
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Xenon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Radium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(U)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
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	-5.60067356E-15	-5.01377045E-15	0.00000000E+00	Charge

539 Solution Parameters, Calculated
540 SOLUTION MASS 461.602144251003 grams
541 H2O MASS 347.563995068949 grams
542 TDS(g/kg) 328.10692108174 g/kgH2O
543
544 Specified Solution Density
545 DENSITY 1188.93254605458 kg/m³ = g/l
546
547 Solution Parameters Based on Specified Density
548 SOLUTION VOL 0.388249228926239 liters
549 TDS 293.724084133903 g/l
550
551 Density based on TDS and NaCl solutions 1188.93254605458 g/l
552 Percent relative error vs NaCl density 0.000000000000000E+000 %
553
554
555
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559

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31822E-01	7.77959E-01	0.9352	1.92928E+01	4.96918E+01	8.95208E+05	
NpO2CO3(s)	9.99922E+00	1.00000E+00	1.000	3.47540E+00	8.95147E+00	3.15133E+06	
Cl-	5.61096E+00	5.29371E-07	0.9434	1.95017E+00	5.02298E+00	1.78080E+05	
Na+	5.61057E+00	5.29268E+00	0.9433	1.95003E+00	5.02263E+00	1.15469E+05	
NpO2+	6.12705E-04	1.21978E-03	1.991	2.12954E-04	5.48499E-04	1.47572E+02	
CO2(aq)	3.86103E-04	1.12115E-03	2.904	1.34196E-04	3.45643E-04	1.52117E+01	
HCO3-	2.26571E-04	8.38810E-05	0.3702	7.87401E-05	2.02829E-04	1.23760E+01	-5.15E-12
H+	1.21872E-06	4.78095E-06	3.923	4.23582E-07	1.09101E-06	1.09962E-03	-2.29E-11
NpO2CO3-	1.33528E-07	2.49717E-07	1.820	4.64090E-08	1.19534E-07	3.93348E-02	1.85E-14
CO3=	3.09384E-08	8.03443E-10	2.59668E-02	1.07531E-08	2.76963E-08	1.66203E-03	1.68E-11
OH-	3.01685E-09	1.63977E-09	0.5435	1.04855E-09	2.70071E-09	4.59318E-05	2.30E-11
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--	1.98384E-11	5.13355E-16	2.5877E-05	6.89511E-12	1.77595E-11	6.80960E-06	1.69E-11
NpO2(OH)2-	2.04311E-16	6.10703E-17	0.2988	7.10356E-17	1.82964E-16	5.54494E-11	1.92E-11
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.02E+01
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.24E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.95E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.91E+00
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+00
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.16E+02
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+00
NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.38E+00

587 pH (-log(aH+)); pOH(-log(mOH+)) 5.3205 5.9141
588 Osmotic Coefficient= 1.241871
589 Equilibrium RH (%) = 77.795863
590 Ionic Strength (m) = 5.611188
591 Density, kg/m3 = 1188.93
592 fCO2(g); log(fCO2(g))= 3.400E-02 -1.47
593
594 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
595 - Gas "molality" and "activity" are gas partial pressures
596 - "Descriptor" means:
597 *G/R/T/ln10 for species with nonzero concs. (convergence criterion)
598 *Saturation Index for minerals, SI=log10(IAP/Ksp)
599 *log10(activity) for aqueous species with very small concentrations
600 *log10(partial pressure) for gases
601
602 Total G/R/T= -4.63379813E+03
603 Flashing Titration # 2
604 # Inversions for batch pblm 19
605 Benchmark TITRATE Problem, LINEAR option: Np(V)O2 with CO2 in 5.61molal NaCl PWT V2.1
606 DATABASE: NWS4/FWS6; Np(V)-Na-CO3-OH-Cl-C1O4 (NR94)
607 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRFR89,FRF90,PP1,RPFR92,RPF94,RRFF94)
608 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
609
610 Elemental Abundances for Flash Problem

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

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736 -1.62342993E-15 -4.66849050E-15 -4.17956521E-15 0.00000000E+00 Charge
737
738 Solution Parameters, Calculated
739 SOLUTION MASS 461.762759746566 grams
740 H2O MASS 347.741937885849 grams
741 TDS (g/kg) 327.889188614766 g/kgH2O
742
743 Specified Solution Density
744 DENSITY 1188.82098252588 kg/m^3 = g/l
745
746 Solution Parameters Based on Specified Density
747 SOLUTION VOL 0.388420768588271 liters
748 TDS 293.549756041959 g/l
749
750 Density based on TDS and NaCl solutions 1188.82098252588 g/l
751 Percent relative error vs NaCl density 0.00000000000000E+000 %
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31857E-01	7.78045E-01	0.9353	1.93027E+01	4.96954E+01	8.95273E+05	
NaHPO2CO3 (s)	9.99481E+00	1.00000E+00	1.000	3.47562E+00	8.94807E+00	3.15013E+06	
Na+	5.61000E+00	5.29001E+00	0.9430	1.95083E+00	5.02247E+00	1.15465E+05	
Cl-	5.60892E+00	5.29003E+00	0.9431	1.95046E+00	5.02151E+00	1.78028E+05	
HCO3-	9.89705E-04	3.66450E-04	0.3703	3.44182E-04	8.86055E-04	5.40645E+01	
CO3=	4.25167E-05	1.10426E-05	2.5972E-02	1.47848E-05	3.80640E-05	2.28419E+00	
CO2(aq)	5.36072E-06	1.55648E-06	2.903	1.86415E-06	4.79930E-06	2.11216E-01	-3.58E-08
OH-	9.49137E-07	5.16005E-07	0.5437	3.30055E-07	8.49735E-07	1.44517E-02	-1.27E-07
HPO2+	4.46247E-07	8.87823E-07	1.990	1.55179E-07	3.99512E-07	1.07407E-01	2.08E-07
HPO2CO3-	1.33612E-07	2.43092E-07	1.819	4.64625E-08	1.19619E-07	3.93614E-02	6.11E-13
HPO2(CO3)2=	2.72677E-08	7.05058E-13	2.5892E-05	9.48213E-09	2.44120E-08	9.49785E-03	-1.46E-07
H+	3.87609E-09	1.51947E-08	3.920	1.34788E-09	3.47015E-09	1.49756E-06	1.59E-07
HPO2(CO3)3=	2.35800E-10	1.86755E-19	7.9201E-10	8.19976E-11	2.11105E-10	9.48020E-05	-2.85E-07
HPO2OH(aq)	1.76865E-10	1.76865E-10	1.000	6.15032E-11	1.58342E-10	4.52944E-05	-1.72E-07
HPO2(OH)2-	1.47303E-14	4.40170E-15	0.2988	5.12234E-15	1.31876E-14	3.99666E-09	-1.77E-07
HCl(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.47E+02
NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.96E+02
HPO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.02E+00
HPO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.62E+00
NaHPO2(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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.31E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.78E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.61E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.10E+00
Na3H(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.40E+00

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812 pH (-log[aH+]); pOH(-log[OH-]) 7.0183 8.4116
813 Gasolite Coefficient= 1.241604
814 Equilibrium RH (%) = 77.804942
815 Ionic Strength (m) = 5.610043
816 Density, kg/m3 = 1188.82
817 fCO2(g); log{fCO2(g)} = 4.720E-04 -3.33

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

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825 Total G/RT= -4.63496201E+03
826 Flashing Titration # 4
827 # inversions for batch phin 22
828 Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61moleal NaCl FMT V2.3
829 DATABASE: NpM84/FW66; Np(V)-Na-CO3-OH-Cl-ClO4 (NRY94);
830 95_01_31 Am(III)-Na-Cl-CO3-2O4-PO4 (FRSR9, FRF9, FRF92, RFF94, RRF94)
831 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin

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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	5.55131618E+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	5.60789978E+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	1.67307744E+01	Carbon
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	Potassium
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
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)
3.4761578E+00	5.5613783E-07	4.97894646E-07	1.18025030E-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	-4.08388619E-15	-3.65619203E-15	0.00000000E+00	Charge

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836 Solution Parameters, Calculated
837 SOLUTION MASS 461.880517078989 grams
838 H2O MASS 347.812004756083 grams
839 TDS (g/kg) 327.883894418751 g/kgH2O
840
841 Specified Solution Density
842 DENSITY 1188.81826953613 kg/m^3 = g/l
843
844 Solution Parameters Based on Specified Density
845 SOLUTION VOL 0.388520709106543 liters
846 TDS 293.545516750385 g/l
847
848 Density based on TDS and NaCl solutions 1188.81826953613 g/l
849 Percent relative error vs NaCl density 0.00000000000000E+000 %
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31863E-01	7.78070E-01	0.9353	1.93077E+01	4.96954E+01	8.95273E+05	
NaHPO2CO3 (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"

Table with columns: Species Name, Molar Concentration, Activity, and other parameters. Includes species like H2O, Na+, Cl-, CO2(aq), and various mineral species like NaH2PO4 and NaHCO3.

pH (-log(aH+)); pOH(-log(aOH+)) 8.9167 9.5098
Osmotic Coefficient* 1.24131
Equilibrium RN (#) = 77.806941
Ionic Strength (M) = 5.610547
Density, kg/m3 = 1188.82
fCO2(g); log(fCO2(g)) = 3.841E-05 -4.43

NOTES: - Water 'molarity' is mole fraction H2O in aqueous phase
- Gas 'molarity' and 'activity' are gas partial pressures
- 'Descriptor' means:
*G/R/T/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/R/T = -4.63554267E+01
Flashing Titration # 5
Inversions for batch phin 23
Benchmark TITRATE Problem, LINEAR option; Hp(V)O2 with CO2 in 5.61molar NaCl FMT V2.1
DATABASE: WMS84/FWS8; Hp(V)-Na-CO2-OH-Cl-C1O4 (RHS4);
SS.01.11 AN(III)-Na-Cl-OH-CO2-OH (FRHS9, FRP90, P91, RPT92, RPT94, RPT94)
Pressure = 1.00000E+00 (=) ATM Temperature = 2.98E+02 (=) Kelvin

Elemental Abundances for Flash Problem

Table with columns: Total Moles, Aq. Molality, Aq. Molarity, Aq. mg/liter, and Descriptor. Lists elements from Hydrogen to Charge with their respective values.

Solution Parameters, Calculated

SOLUTION MASS 461.99831238771 grams
H2O MASS 347.922101921007 grams
TDS (g/kg) 327.878650674697 g/kgH2O

Specified Solution Density

DENSITY 1188.81558239116 kg/m3 = g/l

Solution Parameters based on Specified Density

SOLUTION VOL 0.38862068943010 liters
TDS 293.541317843627 g/l
Density based on TDS and NaCl solutions 1188.81558239116 g/l
Percent relative error vs NaCl density 0.00000000000000E+00 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Table with columns: Species Name, Molality, Activity, Act Coef, Total Moles, Molarity, mg/liter, and Descriptor. Provides detailed concentration data for various species in the batch system.

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

983 pH (-log[am+]); pmi(-log[mi+]) 9.1977 9.7906
984 Osmotic Coefficient= 1.241460
985 Equilibrium RH (%) = 77.608967
986 Ionic strength (m) = 5.611058
987 Density, kg/m3 = 1188.82
988 fCO2(g); log[fCO2(g)] = 2.033E-05 -4.65
989
990 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
991 - Gas "molality" and "activity" are gas partial pressures
992 - "Descriptor" means:
993 *dg/RT/ln10 for species with nonzero concs. (convergence criterion)
994 *saturation index for minerals. SI=log10(IAP/Ksp)
995 *log10(activity) for aqueous species with very small concentrations
996 *log10(partial pressure) for gases
997

998 Total G/RT= -4.63612311E+03
999 Flashing Titration # 6
1000 # Inversions for batch pbm 23
1001 Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
1002 DATABASE: N0M84/PW8; Np(V)-Na-CO3-OH-Cl-C1O4 (NR94);
1003 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFP92,RFP94,RFP94)
1004 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1005

1006 Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.86357676E+01	1.11018428E+02	9.23921088E+01	1.00177306E+05	Hydrogen
1.65884939E+01	5.55164947E+01	4.97025726E+01	7.95211340E+05	Oxygen
5.4279440E+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	1.77929238E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47561744E+00	2.59235443E-03	2.12087229E-03	2.78759970E+01	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PotIion
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NeqIon
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	TracerCl
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
-1.4217169E-15	-4.08525032E-15	-3.65742562E-15	0.00000000E+00	Charge

1034 Solution Parameters, Calculated
1035 SOLUTION MASS 461.11654836857 grams
1036 H2O MASS 348.012201242052 grams
1037 TDS(g/kg) 127.873428539486 g/kgH2O
1038
1039 Specified solution Density
1040 DENSITY 1188.81290631058 kg/m3 = g/l
1041
1042 Solution Parameters Based on Specified Density
1043 SOLUTION VOL. 0.388720674534911 liters
1044 TDS 293.537136225970 g/l
1045
1046 Density based on TDS and NaCl solutions 1188.81290631058 g/l
1047 Percent relative error vs NaCl density 0.000000000000000E+000 %
1048
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1051

1052 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	1.11018428E+02	7.78110E-01	0.9354	3.93177E+01	4.96956E+01	8.95276E+05	
NaHPO2CO3(a)	9.98705E+00	1.00000E+00	1.000	3.47562E+00	8.94116E+00	3.14770E+06	
Na+	5.61000E+00	5.28904E+00	0.9428	1.95235E+00	5.02250E+00	1.15466E+05	
Cl-	5.60582E+00	5.28545E+00	0.9429	1.95089E+00	5.01875E+00	1.77930E+05	
CO3-	1.55719E-03	4.04423E-05	2.5946E-02	5.41999E-04	1.39429E-03	6.36703E+01	
HCO3-	1.03174E-03	3.81899E-04	0.3702	3.59057E-04	9.23688E-04	5.63608E+01	
OH-	3.33488E-05	1.81350E-05	0.5438	1.16058E-05	2.98564E-05	5.07777E-01	
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=	3.14830E-07	2.50542E-16	7.9580E-10	1.09556E-07	2.81860E-07	1.26576E-01	4.15E-08
CO2(aq)	1.58957E-07	4.61543E-07	2.904	5.53190E-08	1.42310E-07	6.26305E-03	-1.04E-07
NpO2CO3-	1.31671E-07	2.43138E-07	1.819	4.65193E-08	1.19672E-07	3.93789E-02	1.02E-12
NpO2-	1.22005E-08	2.42463E-08	1.987	4.24592E-09	1.09228E-08	2.53875E-03	-1.66E-08
NpO2OH(aq)	1.69754E-10	1.69754E-10	1.000	5.90766E-11	1.51977E-10	4.24737E-05	3.26E-08
H+	1.10445E-10	4.32378E-10	2.915	3.84361E-11	9.88785E-11	9.86596E-08	-4.95E-08
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	-3.95E+02
NpO2OH(aq)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.64E+00
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.31E+02
Na3NpO2(CO3)2(s)_DISABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.38E+00
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.21E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.25E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.54E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.61E+00
Na3H(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	

1081 pH (-log[am+]); pmi(-log[mi+]) 9.3641 9.9569
1082 Osmotic Coefficient= 1.241388
1083 Equilibrium RH (%) = 77.810972
1084 Ionic strength (m) = 5.611568
1085 Density, kg/m3 = 1188.81
1086 fCO2(g); log[fCO2(g)] = 1.400E-05 -4.85
1087
1088 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1089 - Gas "molality" and "activity" are gas partial pressures
1090 - "Descriptor" means:
1091 *dg/RT/ln10 for species with nonzero concs. (convergence criterion)
1092 *saturation index for minerals. SI=log10(IAP/Ksp)
1093 *log10(activity) for aqueous species with very small concentrations
1094 *log10(partial pressure) for gases
1095
1096 Total G/RT= -4.63670347E+03
1097 Flashing Titration # 7
1098 # Inversions for batch pbm 23
1099 Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
1100 DATABASE: N0M84/PW8; Np(V)-Na-CO3-OH-Cl-C1O4 (NR94);
1101 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFP92,RFP94,RFP94)
1102 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1103
1104 Elemental Abundances for Flash Problem
1105
1106

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			
3.47697778E+00	3.11028689E+03	2.78456916E+03	3.34454601E+01	Carbon			
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Positron			
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Negitron			
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	C104-(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	-4.58312542E-15	-4.10316801E-15	0.00000000E+00	Charge			
Solution Parameters, Calculated							
SOLUTION MASS	462.233986835158	grams					
H2O MASS	348.102302046915	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 0.000000000000000000 %							
TABLE OF CONCENTRATIONS FOR BATCH SYSTEM							
Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31882E-01	7.78130E-01	0.9354	1.93227E+01	4.96957E+01	8.95277E+05	
NaH2PO4(CO3) (s)	9.98446E+00	1.00000E+00	1.000	3.47562E+00	8.93886E+00	3.14689E+06	
Na+	5.61001E+00	5.28872E+00	0.9427	1.95286E+00	5.02251E+00	1.15466E+05	
Cl-	5.60479E+00	5.28392E+00	0.9428	1.95104E+00	5.01784E+00	1.77897E+05	
CO3=	1.04196E-03	3.85644E-04	0.3701	3.62709E-04	9.32843E-04	5.69194E-01	
OH-	4.37579E-05	2.37975E-05	0.5438	1.52322E-05	3.91755E-05	6.66269E-01	-7.34E-08
NpO2(CO3)2=	1.32081E-06	3.42703E-11	2.5946E-05	4.59777E-07	1.18249E-06	4.60066E-01	5.47E-08
NpO2(CO3)3=	5.51937E-07	4.39934E-16	7.9707E-10	1.92131E-07	4.94137E-07	2.21904E-01	1.21E-07
NpO2CO3-	1.33690E-07	2.43152E-07	1.819	4.65379E-08	1.19690E-07	3.93847E-02	2.67E-12
CO2(aq)	1.22112E-07	1.00000E-07	1.004	4.25802E-08	1.09511E-07	4.81956E-03	-4.08E-07
NpO2	9.21138E-09	1.82991E-08	1.987	3.20650E-09	8.24674E-09	2.21876E-03	-4.64E-08
NpO2OH(aq)	1.68120E-10	1.68120E-10	1.000	5.85229E-11	1.50514E-10	4.30552E-05	1.20E-07
H+	8.42049E-11	3.29505E-10	3.913	2.93119E-11	7.53867E-11	7.59823E-08	-1.70E-07
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)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.49E+02
NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.94E+02
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.05E+00
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.64E+00
Na3HPO4(CO3)2(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.31E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.29E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.09E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.13E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.69E+00
pH (-log(aH+)); pOH(-log(aOH-)) 9.4821 10.0747							
Osmotic Coefficient= 1.241316							
Equilibrium RN (R) = 77.813976							
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":							
*QO/RT/h10 for species with nonzero concn. (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 Q/RT= -4.63728377E+03							
Flashing Titration # 8							
# Inversions for batch plm 24							
Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3							
DATABASE: ION94/F98; Np(V)-Na-CO3-OH-Cl-C104 (SR94)							
95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FASR89, F990, 991, RFP92, RFP94, RFP98)							
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	1.11018449E+02	9.93924776E+01	1.00177678E+05	Hydrogen			
3.67058599E+01	5.55196248E+01	4.97055410E+01	7.95258832E+05	Oxygen			
5.42897768E+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			
1.95118819E+00	5.60752888E+00	5.01692095E+00	1.77864898E+05	Chlorine			
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur			
3.47687811E+00	3.12801754E+03	2.78408705E+03	3.30127736E+01	Carbon			
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Positron			
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Negitron			
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)			
3.4752578E+00	2.43966944E+06	2.16323999E+06	5.62021785E+01	Np(V)			
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	C104-(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			
-7.64531209E-16	-2.19572053E-15	-1.96578196E-15	0.00000000E+00	Charge			

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

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1231 Solution Parameters, Calculated
1232 SOLUTION MASS 462.351826978109 grams
1233 H2O MASS 348.192404119958 grams
1234 TDS(g/kg) 327.863047864827 g/kgH2O
1235
1236 Specified Solution Density
1237 DENSITY 1188.80758671231 kg/m^3 = g/l
1238
1239 Solution Parameters Based on Specified Density
1240 SOLUTION VOL 0.388920656417378 liters
1241 TDS 293.528823873111 g/l
1242
1243 Density based on TDS and NaCl solutions 1188.80758671231 g/l
1244 Percent relative error vs NaCl density 0.00000000000000E+000 %
1245
1246
1247
1248
1249
1250

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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31888E-01	7.78150E-01	0.9354	1.93277E+01	4.96957E+01	8.95279E+05	
NaHPO2CO3(a)	9.98188E+00	1.00000E+00	1.000	3.47561E+00	8.93627E+00	3.14608E+06	
Na+	5.61001E+00	5.28842E+00	0.9427	1.95336E+00	5.02252E+00	1.15467E+05	
Cl-	5.60375E+00	5.28239E+00	0.9427	1.95118E+00	5.01692E+00	1.77865E+05	
CO3=	2.56997E-03	6.67295E-05	2.5965E-02	8.94845E-04	2.30084E-03	1.38072E+02	
HCO3-	1.05192E-03	3.85206E-04	0.3701	3.66285E-04	9.41799E-04	5.74658E+01	
OH-	5.39719E-05	2.93547E-05	0.5439	1.87926E-05	4.83199E-05	8.21791E-01	-4.00E-09
NpO2(CO3)2=	1.64391E-06	4.26761E-11	2.5960E-05	5.72396E-07	1.47176E-06	5.72609E-01	1.61E-08
NpO2(CO3)3=	8.54848E-07	6.82175E-16	7.9835E-10	2.97525E-07	7.65001E-07	3.43543E-01	3.23E-08
NpO2CO3-	1.33710E-07	2.43167E-07	1.819	4.65568E-08	1.19708E-07	3.93906E-02	7.87E-12
CO2(aq)	1.00104E-07	2.90667E-07	2.904	3.48556E-08	8.96214E-08	3.94422E-03	-9.97E-08
NpO2	7.40067E-09	1.46965E-08	1.986	2.57685E-09	6.63567E-09	1.78262E-03	-1.60E-08
NpO2OH(aq)	1.65553E-10	1.65553E-10	1.000	5.79923E-11	1.49111E-10	4.26538E-05	3.82E-08
H+	6.82959E-11	2.67131E-10	3.911	2.37801E-11	6.11438E-11	6.16269E-08	-5.42E-08
NpO2(OH)2-	7.89467E-13	2.35806E-13	0.2987	2.74886E-13	7.06793E-13	1.24202E-07	9.25E-08
NCl(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.94E+02
NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.94E+02
NpO2OH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.05E+00
NpO2OH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.44E+00
Na3NpO2(CO3)2(s) DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.31E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.28E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.99E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.32E+00
Na3H(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.59E+00

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1280 pH (-log[aH+]); pOH(-log[OH-]) 9.5733 10.1656
1281 Osmotic Coefficient= 1.241245
1282 Equilibrium RH (%) = 77.814978
1283 Tonic Strength (m) = 5.61232
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 *00/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 pbm 29
1298 Benchmark TITRATE Problem. LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
1299 DATABASE: RMW84/PWS6; Np(V)-Na-CO3-OH-Cl-C1O4 (NR94);
1300 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,FRF90,P91,RFRF92,RFF94,RRF94)
1301 Pressure= 1.00000E+00 [atm] Temperature= 2.98E+02 [=] Kelvin
1302
1303 Elemental Abundances for Flash Problem
1304
1305
1306

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Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.86657977E+01	1.11018489E+02	9.93926605E+01	1.00177862E+05	Hydrogen
3.47151119E+01	5.55211888E+01	4.97070238E+01	7.95282556E+05	Oxygen
5.42948290E+00	5.61000979E+00	5.02251097E+00	1.15466832E+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
1.95132336E+00	5.60271996E+00	5.01600453E+00	1.77832409E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47705844E+00	4.1454576E-03	3.71142525E-03	4.4577286E+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	3.32866843E-06	2.98091111E-06	7.06425232E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	C1O4-[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
-1.15045794E-15	-3.30323204E-15	-2.95731840E-15	0.00000000E+00	Charge

```

1331 Solution Parameters, Calculated
1332 SOLUTION MASS 462.469675148448 grams
1333 H2O MASS 348.28250731911 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 0.38920652869917 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 0.00000000000000E+000 %
1345
1346
1347
1348
1349
1350

```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31895E-01	7.78170E-01	0.9354	1.93277E+01	4.96958E+01	8.95280E+05	
NaHPO2CO3(a)	9.97930E+00	1.00000E+00	1.000	3.47561E+00	8.93627E+00	3.14527E+06	
Na+	5.61001E+00	5.28810E+00	0.9424	1.95307E+00	5.02253E+00	1.15467E+05	

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```

1355 Cl-          Cl-          5.60272E+00  5.20086E+00  0.9426      1.95133E+00  5.01600E+00  1.77832E+05
1356 CO3=        CO3=        3.07597E-03  7.98610E-05  2.5964E-02  1.07131E-03  2.75385E-03  1.65256E+02
1357 HCO3=       HCO3=       1.06176E-03  3.92894E-04  0.3700      3.69799E-04  9.50572E-04  5.80012E+01
1358 OH-         OH-         6.40010E-05  3.46124E-05  0.5439      2.22304E-05  5.72980E-05  9.74498E-01
1359 HPO2(CO3)2= HPO2(CO3)2= 1.96453E-04  5.10785E-11  2.5974E-05  6.84909E-07  1.74000E-06  6.84909E-01
1360 HPO2(CO3)3= HPO2(CO3)3= 1.22205E-06  9.77145E-16  7.9962E-10  4.25620E-07  1.09408E-06  4.91324E-01
1361 HPO2CO3=    HPO2CO3=    1.33729E-07  2.43181E-07  1.818      4.65756E-08  1.19725E-07  3.93944E-02
1362 CO2(aq)     CO2(aq)     8.51877E-08  2.47357E-07  2.904      2.96694E-08  7.62669E-08  3.35649E-03
1363 HPO2OH(aq)  HPO2OH(aq)  6.18610E-09  1.22804E-08  1.985      2.15458E-09  5.53847E-09  1.49011E-03
1364 HPO2OH(amor) HPO2OH(amor) 1.45046E-10  1.65045E-10  1.000      5.74825E-11  1.47762E-10  4.22680E-05
1365 H+          H+          5.76161E-11  2.25288E-10  3.910      2.00667E-11  5.15926E-11  5.19010E-08
1366 HPO2(OH)2= HPO2(OH)2= 9.27855E-13  2.71117E-13  0.2987     3.23156E-13  8.10690E-13  2.51750E-07
1367 HCl(aq).....to.titrant.acid.only  0.00000E+00  0.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1368 NaOH(aq).....to.titrant.base.only  0.00000E+00  0.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1369 HPO2OH(aged) HPO2OH(aged) 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1370 HPO2OH(amor) HPO2OH(amor) 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1371 Na3HPO2(CO3)2(s) Na3HPO2(CO3)2(s) 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1372 NaCl         NaCl         0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1373 NaHCO3      NaHCO3      0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1374 Na2CO3.10H2O Na2CO3.10H2O 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1375 Na2CO3.7H2O Na2CO3.7H2O 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1376 Na2CO3.H2O  Na2CO3.H2O  0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1377 Na3H(CO3)2.2H2O Na3H(CO3)2.2H2O 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1378
1379 pH (-log[M+]); pM(-log[M-])      9.6473      10.2395
1380 Osmotic Coefficient=            1.241173
1381 Equilibrium RH (%) =            77.816979
1382 Ionic Strength (m) =            5.613104
1383 Density, kg/m3 =                1188.80
1384 fCO2(g), log[fCO2(g)] =              7.501E-06  -5.13
1385
1386 NOTES: - Water 'molarity' is mole fraction H2O in aqueous phase
1387         - Gas 'molarity' and 'activity' are gas partial pressures
1388         - 'Descriptor' means:
1389           *G/RT/ln10 for species with nonzero comps. (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= -4.6304423E+03
1395 Flashing Titration #            10
1396 # Inversions for batch phm      29
1397 Benchmark TITRATE Problem, LINEAR option; Hp(VI)O2 with CO3 in 5.61molal NaCl PWT V2.1
1398 DATABASE: H0N84/PW86; Hp(VI)-Na-CO3-ON-Cl-C1O4 (H094);
1399 95.01.11 Am(III)-Na-Cl-CO3-ED4-PO4 (FR889,FR930,P91,RFF92,RFF94,KRFF94)
1400 Pressure= 1.00000E+00 (s) ATM Temperature= 2.98E+02 (s) Kelvin
1401
1402 Elemental Abundances for Flash Problem
1403
1404 Total Moles      Aq. Molarity      Aq. Molarity      Aq. mg/liter
1405
1406 3.86758077E+01  1.11018508E+02  9.93928423E+01  1.00178046E+05  Hydrogen
1407 3.67206779E+01  5.55227521E+01  4.97085056E+01  4.97085056E+05  Oxygen
1408 5.42980892E+00  5.61001000E+00  5.61001000E+00  5.61001000E+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 1.95147452E+00  5.60168756E+00  5.01508853E+00  1.77799934E+05  Chlorine
1413 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Sulfur
1414 3.47723877E+00  4.56281109E-01  4.17453320E-03  5.01492000E-01  Carbon
1415 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Phosphorus
1416 0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00  Nitrogen
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  Tracer:Zl
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  4.08213591E-06  3.65466170E-06  8.66310978E-01  Hp(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 -1.76219826E-15 -5.05837199E-15 -4.52866803E-15 0.00000000E+00 Charge
1429
1430 Solution Parameters, Calculated
1431 SOLUTION MASS 462.587531269118 grams
1432 H2O MASS 348.372611719453 grams
1433 TDS(g/kg) 327.852752218200 g/kgH2O
1434
1435 Specified Solution Density
1436 DENSITY 1188.80231065170 kg/m3 = g/l
1437
1438 Solution Parameters Based on Specified Density
1439 SOLUTION VOL 0.389120651782 liters
1440 TDS 293.520579551782 g/l
1441
1442 Density based on TDS and NaCl solutions 1188.80231065170 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         8.31901E-01  7.78190E-01  0.9354      1.93377E+01  4.96959E+01  8.95282E+05
1452 Na3HPO2CO3(s)   Na3HPO2CO3(s) 9.97672E+00  1.00000E+00  1.000      3.47561E+00  8.93197E+00  3.14446E+06
1453 Na+             Na+           5.61001E+00  5.28779E+00  0.9426      1.95437E+00  5.02254E+00  1.35667E+05
1454 Cl-             Cl-           5.60169E+00  5.27933E+00  0.9425      1.95147E+00  5.01509E+00  1.77800E+05
1455 CO3=           CO3=         3.58175E-03  9.29893E-05  2.5962E-02  1.24778E-03  3.20687E-03  1.92430E+02
1456 HCO3=          HCO3=        1.07131E-03  3.96412E-04  0.3700      3.73239E-04  9.59185E-04  5.85267E+01
1457 OH-            OH-          6.40010E-05  3.46124E-05  0.5439      2.57289E-05  6.61206E-05  1.2453E+00
1458 HPO2(CO3)2=    HPO2(CO3)2= 2.28868E-06  9.94773E-11  2.5988E-05  7.97312E-07  2.04901E-06  7.87199E-01
1459 HPO2(CO3)3=    HPO2(CO3)3= 1.65423E-06  1.32488E-15  0.0090E-10  5.76289E-07  1.48100E-06  6.65081E-02
1460 HPO2CO3=       HPO2CO3=     1.33749E-07  2.43195E-07  1.818      4.65945E-08  1.19743E-07  3.94922E-02
1461 CO2(aq)        CO2(aq)      7.44762E-08  2.16257E-07  2.904      2.59455E-08  6.66772E-08  2.93445E-03
1462 H+             H+           5.76161E-11  1.05475E-08  1.984      1.85172E-09  4.75872E-09  1.28032E-03
1463 HPO2OH(aq)     HPO2OH(aq)  1.51533E-09  1.63595E-10  1.000      5.69919E-11  1.46443E-10  4.18946E-05
1464 H+             H+           4.99485E-11  1.95194E-10  3.908      1.74007E-11  4.47180E-11  4.50712E-08
1465 HPO2(OH)2=    HPO2(OH)2=  1.06147E-12  3.16997E-13  0.2986     3.69789E-13  9.50319E-13  2.88005E-07
1466 HCl(aq).....to.titrant.acid.only  0.00000E+00  0.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1467 NaOH(aq).....to.titrant.base.only  0.00000E+00  0.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1468 HPO2OH(aged)  HPO2OH(aged) 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1469 HPO2OH(amor)  HPO2OH(amor) 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1470 Na3HPO2(CO3)2(s) Na3HPO2(CO3)2(s) 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1471 NaCl           NaCl         0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1472 NaHCO3        NaHCO3      0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1473 Na2CO3.10H2O  Na2CO3.10H2O 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1474 Na2CO3.7H2O  Na2CO3.7H2O  0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1475 Na2CO3.H2O   Na2CO3.H2O  0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1476 Na3H(CO3)2.2H2O Na3H(CO3)2.2H2O 0.00000E+00  1.00000E+00  1.000      0.00000E+00  0.00000E+00  0.00000E+00
1477
1478 pH (-log[M+]); pM(-log[M-])      9.7095      10.3015

```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

1479 Osmotic Coefficient= 1.241102
1480 Equilibrium RH (%) = 77.81880
1481 Ionic Strength (m) = 5.613617
1482 Density, kg/ml = 1188.80
1483 fCO2(g); log{fCO2(g)}= 6.558E-06 -5.18
1484
1485 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1486 - Gas "molality" and "activity" are gas partial pressures
1487 - "Descriptor" means:
1488 *CG/RT/ln10 for species with nonzero concs. (convergence criterion)
1489 *saturation index for minerals, SI=log10(IAP/Ksp)
1490 *log10(activity) for aqueous species with very small concentrations
1491 *log10(partial pressure) for gases
1492
1493 Total G/RT= -4.63902442E+03
1494 Flashing Titration # 11
1495 # inversions for batch pbm 29
1496 benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
1497 DATABASE: IOM984/PW86; Np(V)-Na-CO3-OH-Cl-C104 (NR94);
1498 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,PF1,RFFR92,RFF94,RFF94)
1499 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1500

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1.86858177E+01	1.11018527E+02	9.93930312E+01	1.00178222E+05	Hydrogen
1.67262240E+01	5.55243148E+01	4.97098664E+01	7.95129558E+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
1.95161989E+00	5.60065587E+00	5.01417296E+00	1.77767474E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47741911E+00	5.17999117E+03	4.63756089E+03	5.57017439E+01	Carbon
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	Nitrogen
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#1
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	4.89951732E+06	4.38645561E+06	1.03980141E+00	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4- (L)
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	-4.10249989E-15	0.00000000E+00	Charge

Solution Parameters, Calculated

SOLUTION MASS	462.705392781822	grams
H2O MASS	348.462717099515	grams
TDS(g/kg)	327.847636411822	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 solution	0.000000000000000E+000	%

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31907E-01	7.78210E-01	0.9355	1.93427E+01	4.96960E+01	8.95203E+05	
NaH2PO2CO3(a)	9.37413E+00	1.00000E+00	1.000	2.47561E+00	8.92968E+00	1.14366E+06	
Na+	5.61001E+00	5.28749E+00	0.9425	1.95488E+00	5.02255E+00	1.15467E+05	
Cl-	5.60066E+00	5.27780E+00	0.9424	1.95162E+00	5.01417E+00	1.77767E+05	
CO3=	4.08730E-03	1.06108E-04	2.5960E-02	1.42427E-03	3.65929E-03	2.19591E+02	
HCO3-	1.08082E-03	3.39846E-04	0.3700	3.76626E-04	9.67642E-04	5.90427E+01	
OH-	8.35418E-05	4.54485E-05	0.5440	2.91110E-05	7.47929E-05	1.27203E+00	-2.32E-10
NpO2(CO3)2=	2.61033E-06	6.78722E-11	2.6001E-05	9.09603E-07	2.33699E-06	9.09240E-01	1.35E-09
NpO2(CO3)3=	2.15059E-06	1.72518E-15	8.0219E-10	7.49402E-07	1.92539E-06	8.64644E-01	2.95E-09
NpO2CO3-	1.33768E-07	2.43209E-07	1.810	4.66133E-08	1.19761E-07	3.94080E-02	6.21E-13
CO2(aq)	6.64082E-08	1.92811E-07	2.904	2.31408E-08	5.94541E-08	2.61856E+03	-1.26E-08
NpO2=	4.66017E-09	9.24400E-09	1.984	1.62190E-09	4.17217E-09	1.12251E-03	-1.34E-09
NpO2OH(aq)	1.62195E-10	1.62195E-10	1.000	5.65189E-11	1.45210E-10	4.15381E-05	5.50E-09
H+	4.41741E-11	1.72551E-10	3.906	1.53930E-11	1.95483E-11	3.98608E-08	-6.05E-09
NpO2(OH)2-	1.19043E-12	3.55535E-13	0.2986	4.14889E-13	1.06595E-12	1.23048E-07	1.24E-08
NCl(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(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.06E+00
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.66E+00
Na1NpO2(CO3)2(a) DISABLED DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.31E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.25E+01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.27E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.79E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.83E+00
NaHCO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.12E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.38E+00

1577 pH (-log{aH+}); pOH(-log{aOH-}) 9.7631 10.3548
1578 Osmotic Coefficient= 1.241102
1579 Equilibrium RH (%) = 77.820979
1580 Ionic Strength (m) = 5.611330
1581 Density, kg/ml = 1188.80
1582 fCO2(g); log{fCO2(g)}= 5.848E-06 -5.23
1583
1584 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1585 - Gas "molality" and "activity" are gas partial pressures
1586 - "Descriptor" means:
1587 *CG/RT/ln10 for species with nonzero concs. (convergence criterion)
1588 *saturation index for minerals, SI=log10(IAP/Ksp)
1589 *log10(activity) for aqueous species with very small concentrations
1590 *log10(partial pressure) for gases
1591

1592 Total G/RT= -4.6390458E+03
1593 Flashing Titration # 12
1594 # inversions for batch pbm 29
1595 benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
1596 DATABASE: IOM984/PW86; Np(V)-Na-CO3-OH-Cl-C104 (NR94);
1597 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,PF1,RFFR92,RFF94,RFF94)
1598 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1599

Elemental Abundances for Flash Problem

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

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```

1603 3.86958278E+01 1.11018546E+02 9.93932031E+01 1.00178409E+05 Hydrogen
1604 3.67317700E+01 5.5528769E+01 4.97114666E+01 7.95353639E+05 Oxygen
1605 5.43100040E+00 5.61001519E+00 5.02258021E+00 1.15487513E+05 Sodium
1606 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1607 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
1608 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
1609 1.9517648E+00 5.59962430E+00 5.0125782E+00 1.77735029E+05 Chlorine
1610 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1611 3.4775984E+00 5.49891170E+01 5.10035774E+03 6.12603968E+01 Carbon
1612 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 PosIon
1613 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 NegIon
1614 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Air
1615 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron
1616 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bromine
1617 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 TracerEl
1618 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Th(IV)
1619 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Am(III)
1620 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 U(VI)
1621 3.4756157E+00 5.78031356E+06 5.17502615E+06 1.22673063E+00 Np(V)
1622 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 ClO4- (EL)
1623 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1624 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Electron
1625 -1.60809713E-15 -4.61363967E-15 -4.13052089E-15 0.00000000E+00 Charge
1626
1627
1628 Solution Parameters, Calculated
1629 SOLUTION MASS 462.823267120614 grams
1630 H2O MASS 348.552823457537 grams
1631 TDS (g/kg) 327.842541998512 g/kgQO
1632
1633 Specified Solution Density
1634 DENSITY 1188.79707833404 kg/m^3 = g/l
1635
1636 Solution Parameters Based on Specified Density
1637 SOLUTION VOL 0.389320663345848 liters
1638 TDS 393.512403582768 g/l
1639
1640 Density based on TDS and NaCl solutions 1188.79707833404 g/l
1641 Percent relative error vs NaCl density 0.000000000000000E+00 %
1642
1643
1644 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1645
1646 Species Name Molality Activity Act Coef Total Moles Molarity mg/liter Descriptor
1647
1648 H2O WATER 8.31913E-01 7.78230E-01 0.9355 1.93477E+01 4.96961E+01 8.95285E+05
1649 NaHPO2CO3(s) NaHPO2CO3(aq) 9.37150E-01 9.37150E-01 0.9355 1.93477E+01 4.96961E+01 8.95285E+05
1650 Na+ Na+ 5.61002E+00 5.28718E+00 0.9425 1.95539E+00 5.02258E+00 1.15488E+05
1651 Cl- Cl- 5.59962E+00 5.27626E+00 0.9423 1.95176E+00 5.01258E+00 1.77735E+05
1652 CO3+ CO3+ 4.59262E-03 1.19219E-04 2.5959E-02 1.60077E-03 4.11170E-03 2.46740E+02
1653 HCO3- HCO3- 1.09010E-01 4.03260E-04 0.1699 3.79959E-04 9.75954E-04 5.95499E+01
1654 OH- OH- 9.30887E-05 5.06260E-05 0.5441 3.24393E-05 8.33230E-05 1.42170E+00 -1.82E-10
1655 NpO2(CO3)2-- NpO2(CO3)2-- 2.93150E-06 7.42632E-11 2.6015E-05 1.02178E-06 2.62452E-06 1.02111E+00 1.03E-09
1656 NpO2(CO3)3--- NpO2(CO3)3--- 2.71072E-06 2.17799E-15 8.0478E-10 4.44829E-07 2.42687E-06 1.08944E+00 2.18E-09
1657 NpO2CO3- NpO2CO3- 1.33788E-07 2.43223E-07 1.818 4.66322E-08 1.19778E-07 3.94138E-02 6.48E-13
1658 CO2(aq) CO2(aq) 6.01101E-08 1.74545E-07 2.904 2.09515E-08 5.38156E-08 2.36842E-03 -1.06E-08
1659 NpO2+ NpO2+ 4.14945E-09 8.22786E-09 1.983 1.44630E-09 3.71494E-09 9.99493E-04 -1.03E-09
1660 NpO2OH(aq) NpO2OH(aq) 1.60844E-10 1.40844E-10 1.000 5.60525E-11 1.44001E-10 4.11921E-05 4.70E-09
1661 H+ H+ 3.96673E-11 5.8878E-10 3.904 1.38262E-11 3.55135E-11 3.57941E-08 -5.71E-09
1662 NpO2(OH)2- NpO2(OH)2- 1.11559E-12 3.92815E-13 0.2986 4.58552E-13 1.17783E-12 3.56954E-07 1.04E-08
1663 HCl(aq).....to titrate.acid only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.49E+02
1664 NaOH(aq).....to titrate.bas only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.94E+02
1665 NpO2OH(aq) NpO2OH(aq) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.07E+00
1666 NpO2OH(amor) NpO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.66E+00
1667 Na3HPO2(CO3)2(a) DISABLED DISABLED 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -9.31E+02
1668 NaCl Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.25E+01
1669 NaHCO3 NaHcolite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.27E+00
1670 Na2CO3.10H2O Nastron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.74E+00
1671 Na2CO3.7H2O Na2CO3-Heptahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.78E+00
1672 Na2CO3.H2O Thermonatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.07E+00
1673 NaH(CO3)2.2H2O Trona 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -4.32E+00
1674
1675 pH (-log[ah+]), pmH(-log[ah+]) 9.8100 10.4016
1676 Osmotic Coefficient= 1.240960
1677 Equilibrium RH (%) = 77.822977
1678 Ionic Strength (m) = 5.614644
1679 Density, kg/m3 = 1188.80
1680 fCO2(g); log(fCO2(g))= 5.293E-06 -5.28
1681
1682 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1683 - Gas "molality" and "activity" are gas partial pressures
1684 - "Descriptor" means:
1685 * "aq/RT/ln10" for species with nonzero concs. (convergence criterion)
1686 * "saturation index" for minerals (SI=ln(IAP/Ksp))
1687 * "log10(activity)" for aqueous species with very small concentrations
1688 * "log10(partial pressure)" for gases
1689
1690 Total G/RT= -4.64018472E+01
1691 Flashing Titration # 11
1692 # Inversions for batch pbm 29
1693 Benchmark TITRATE Problem. LINEAR option: Np(V)O2 with CO3 in 5.6molal NaCl FMT V2.3
1694 DATABASE: IOWB4/FWB6; Np(V)-Na-CO3-OR-Cl-ClO4 (RR94);
1695 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RPFR92,RUFF94,RUFF94)
1696 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1697
1698 Elemental Abundances for Flash Problem
1699
1700 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
1701
1702 3.87058378E+01 1.11018546E+02 9.93932020E+01 1.00178590E+05 Hydrogen
1703 3.67373160E+01 5.55274383E+01 4.97129457E+01 7.95377304E+05 Oxygen
1704 5.43100023E+00 5.61001708E+00 5.02257052E+00 1.15487513E+05 Sodium
1705 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1706 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
1707 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
1708 1.95191003E+00 5.59859345E+00 5.01234310E+00 1.77702600E+05 Chlorine
1709 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1710 3.47777977E+00 5.21362642E+03 5.56297360E+03 6.8168759E+01 Carbon
1711 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 PosIon
1712 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 NegIon
1713 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Air
1714 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron
1715 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bromine
1716 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 TracerEl
1717 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Th(IV)
1718 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Am(III)
1719 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 U(VI)
1720 3.4756157E+00 6.72405267E+06 6.01995114E+06 1.42701858E+00 Np(V)
1721 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 ClO4- (EL)
1722 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1723 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Electron
1724 -1.01284388E-15 -2.90539042E-15 -2.60115577E-15 0.00000000E+00 Charge
1725
1726

```


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) 127.837468998058 g/kgH2O
1731
1732 Specified Solution Density
1733 DENSITY 1188.79447861716 kg/m3 = 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 %
```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31920E-01	7.78250E-01	0.9355	1.83527E+01	4.96962E+01	8.95286E+05	
NaHPO2CO3(a)	3.96898E+00	1.00000E+00	1.000	3.47561E+00	8.92509E+00	3.14204E+06	
Na+	5.61002E+00	5.28688E+00	0.9424	1.95589E+00	5.02257E+00	1.15468E+05	
Cl-	5.59559E+00	5.27473E+00	0.9422	1.95191E+00	5.01234E+00	1.17703E+05	
CO3 ²⁻	5.09770E-03	1.32331E-04	2.5957E-02	1.77728E-03	4.56390E-03	2.73874E+02	
HCO3-	1.09923E-03	4.06595E-04	0.3699	3.83240E-04	9.84128E-04	6.00486E+01	
OH-	1.02445E-04	5.57417E-05	0.5441	3.57166E-05	9.17172E-05	1.55986E+00	-1.54E-10
NpO2(CO3)3==	3.33418E-06	2.68321E-15	8.0476E-10	1.16244E-06	2.98505E-06	1.34051E+00	1.71E-09
NpO2(CO3)2==	3.25216E-06	8.46501E-11	2.6029E-05	1.13384E-06	2.91162E-06	1.13281E+00	7.96E-10
NpO2CO3-	1.33807E-07	2.43237E-07	1.818	4.66510E-08	1.19796E-07	3.94196E-02	5.37E-13
CO2(aq)	5.5052E-08	1.59869E-07	2.904	1.91846E-08	4.82902E-08	2.16925E-03	-9.11E-09
NpO2+	3.74015E-09	7.41351E-09	1.982	1.30198E-09	3.34851E-09	9.00905E-04	-7.82E-10
NpO2OH(aq)	1.59537E-10	1.59537E-10	1.000	5.56216E-11	1.42832E-10	4.08576E-05	4.10E-09
H+	3.60509E-11	1.40695E-10	3.903	1.25689E-11	3.23759E-11	3.25108E-08	-4.88E-09
NpO2(OH)2-	1.43661E-12	4.28912E-13	0.2986	5.00864E-13	1.28618E-12	3.89791E-07	8.98E-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(aq).....to titrate.amor	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.07E+00
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.65E+00
NaH2PO2(CO3)2(a) DISABLED DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.31E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.25E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.26E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.70E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.73E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.02E+00
Na3H(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.27E+00

```
1775 pH (-log(aH+)) pmH(-log(aH+)) 9.8517 10.4431
1776 Osmotic Coefficient= 1.240888
1777 Equilibrium RH (%) = 77.824974
1778 Tonic Strength (m) = 5.615154
1779 Density, kg/m3 = 1188.79
1780 fCO2(g): log(fCO2(g)) = 4.848E-06 -5.33
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 *cg/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 pbm 29
1793 Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
1794 DATABASE: NMB4/FW8; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1795 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RPFR92,RPFR94,RRFP94)
1796 Pressure= 1.00000E+00 [atm] Temperature= 2.98E+02 [K] 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 3.47421820E+01 5.55289891E+01 4.97144219E+01 7.95400954E+05 Oxygen
1804 5.43201204E+00 5.61001802E+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 5.59756311E+00 5.01143881E+00 1.17767018E+05 Chlorine
1809 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1810 3.47796010E+00 6.73013708E-03 6.02540823E-03 7.23711783E+01 Carbon
1811 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Positron
1812 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Helium
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 Th(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
```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31926E-01	7.78270E-01	0.9355	1.83577E+01	4.96962E+01	8.95288E+05	
NaHPO2CO3(a)	3.96640E+00	1.00000E+00	1.000	3.47561E+00	8.92279E+00	3.14123E+06	
Na+	5.61002E+00	5.28658E+00	0.9423	1.95640E+00	5.02258E+00	1.15468E+05	
Cl-	5.59559E+00	5.27320E+00	0.9421	1.95206E+00	5.01143E+00	1.17767E+05	

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```

1851 CO3=          CO3=          5.60253E-03  1.45418E-04  2.5956E-02  1.95379E-03  5.01588E-03  3.00999E+02
1852 HCO3=        HCO3=          1.10822E-03  4.09875E-04  0.3499      3.86471E-04  9.92171E-04  6.05394E+01
1853 OH=          OH=          1.1874E-04  6.07695E-05  0.5442      3.89450E-05  9.99819E-05  1.61647E+00
1854 NpO2(CO3)3== NpO2(CO3)3== 4.02056E-06  3.24077E-15  8.0605E-10  1.40210E-06  3.59956E-06  1.3147E+00
1855 NpO2(CO3)2== NpO2(CO3)2== 3.57233E-06  3.30328E-11  2.6043E-05  1.24579E-06  3.19826E-06  1.24433E+00
1856 NpO2CO3=     NpO2CO3=     1.31827E-07  2.43251E-07  1.818       4.66698E-08  1.19813E-07  3.94254E-02
1857 CO2(aq)      CO2(aq)      5.09071E-08  1.47825E-07  2.904       1.77530E-08  4.55765E-08  2.00581E-03
1858 NpO2=        NpO2=        3.40480E-09  6.74629E-09  1.981       1.18737E-09  3.04827E-09  8.20129E-04
1859 NpO2OH(aq)   NpO2OH(aq)   1.58274E-10  1.58274E-10  1.000       5.51952E-11  1.41700E-10  4.05340E-05
1860 H+           H+           3.00838E-11  1.29058E-10  3.901       1.15374E-11  2.96195E-11  2.98535E-08
1861 NpO2(OH)2=  NpO2(OH)2=  1.55392E-12  4.63895E-13  0.2985     5.41903E-13  1.39121E-12  3.12121E-07
1862 HCl(aq).....to.titrate.acid.only  0.00000E+00  0.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1863 NaOH(aq).....to.titrate.basess.only  0.00000E+00  0.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1864 NpO2OH(aq)   NpO2OH(aq)   0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1865 NpO2OH(amor) NpO2OH(amor) 0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1866 NaH2PO2(CO3)2(s)DISABLED_DISABLED  0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1867 NaCl         NaCl         0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1868 NaHCO3       NaHCO3      0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1869 Na2CO3.10H2O Na2CO3.10H2O 0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1870 Na2CO3.7H2O  Na2CO3.7H2O 0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1871 Na2CO3.H2O   Na2CO3.H2O  0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1872 Na3H(CO3)2.2H2O Na3H(CO3)2.2H2O 0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00
1873
1874 pH (-log(aH+)); pOH(-log(aOH+)) 9.8892  10.4804
1875 Osmotic Coefficient= 1.240817
1876 Equilibrium RH (%) = 77.826970
1877 Ionic Strength (m) = 5.615672
1878 Density, kg/m3 = 1189.79
1879 fCO2(g); log(fCO2(g)) = 4.483E-06 -5.35
1880
1881 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1882 - Gas "molality" and "activity" are gas partial pressures
1883 - "Descriptor" means:
1884 *dd/RT/n10 for species with nonzero concs. (convergence criterion)
1885 *saturation index for minerals; E=log10(IAP/Ksp)
1886 *log10(activity) for aqueous species with very small concentrations
1887 *log10(partial pressure) for gases
1888
1889 Total G/RT= -4.64134493E+03
1890 # InverseLog for batch pblm 15
1891 # InverseLog for batch pblm 39
1892 Benchmark TITRATE Problem: LINEAR option: Np(V)O2 with CO3 in 5.6molar NaCl FMT V2.1
1893 DATABASE: IOW84/FW86; Np(V)-Na-CO3-OH-Cl-C104 (NR94);
1894 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,FRP90,PS1,RFFR92,RFP94,RFFP94)
1895 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
1896
1897 Element Abundances for Flash Problem
1898
1899 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
1900
1901 3.87258579E+01 1.11018601E+02 9.93937371E+01 1.00178948E+05 Hydrogen
1902 1.67484080E+01 5.55305529E+01 4.87159013E+01 7.95424591E+05 Oxygen
1903 5.43251790E+00 5.61002101E+00 5.02259074E+00 1.15468197E+05 Sodium
1904 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1905 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
1906 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
1907 1.95220016E+00 5.59653130E+00 5.10514952E+00 1.77637786E+05 Chlorine
1908 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1909 3.47814044E+00 7.24644343E-03 6.48766141E-03 7.92331012E+01 Carbon
1910 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1911 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron
1912 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Nitrogen
1913 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Air
1914 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bromine
1915 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Tracer#1
1916 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Th(IV)
1917 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Am(III)
1918 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 U(VI)
1919 3.47561578E+00 8.79854005E-06 7.87723651E-06 1.86728474E+00 Np(V)
1920 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 ClO4(-EL)
1921 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1922 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Electron
1923 -1.76476943E-15 -5.05920963E-15 -4.52945495E-15 0.00000000E+00 Charge
1924
1925 Solution Parameters, Calculated
1926 SOLUTION MASS 463.176929136620 grams
1927 H2O MASS 348.823147935355 grams
1928 TDS(g/kg) 327.827387253719 g/kgH2O
1929
1930 Specified Solution Density
1931 DENSITY 1188.78931208719 kg/m3 = g/l
1932
1933 Solution Parameters Based on Specified Density
1934 SOLUTION VOL 0.389620704381509 liters
1935 TDS 293.500266120485 g/l
1936
1937 Density based on TDS and NaCl solutions 1188.78931208719 g/l
1938 Percent relative error vs NaCl density 0.000000000000000E+00 %
1939
1940
1941 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1942
1943 Species Name Molality Activity Act Coef Total Moles Molality mg/liter Descriptor
1944
1945 H2O WATER 8.31932E-01 7.78290E-01 0.9355 1.93627E+01 4.96963E+01 8.95289E+05
1946 NaH2PO2CO3(s) NaH2PO2CO3(s) 9.96382E-00 1.00000E+00 1.000 3.47561E+00 8.92050E+00 3.14043E+06
1947 H+ Na+ 5.61002E+00 5.28628E+00 0.9423 1.95991E+00 5.02259E+00 1.15468E+05
1948 Cl- Cl- 5.59653E+00 5.27166E+00 0.9420 1.95220E+00 5.01051E+00 1.77638E+05
1949 CO3= CO3= 6.10711E-03 1.58505E-04 2.5954E-02 2.13010E-03 5.46763E-03 3.28108E+02
1950 HCO3= HCO3= 1.11706E-03 4.13103E-04 0.1698 3.89655E-04 1.00009E-03 6.10225E+01
1951 OH= OH= 1.20768E-04 6.57227E-05 0.5442 4.21267E-05 1.08122E-04 1.83887E+00
1952 NpO2(CO3)3== NpO2(CO3)3== 4.78942E-06 3.85055E-15 8.0734E-10 1.66368E-06 4.27001E-06 1.91755E+00
1953 NpO2(CO3)2== NpO2(CO3)2== 3.89199E-06 1.01411E-10 2.6056E-05 1.35763E-06 3.48466E-06 1.35568E+00
1954 NpO2CO3= NpO2CO3= 1.33844E-07 2.43265E-07 1.817 4.6687E-08 1.19831E-07 3.94312E-02
1955 CO2(aq) CO2(aq) 1.47407E-08 1.37761E-07 2.904 1.65484E-08 4.24731E-08 1.86923E-03
1956 NpO2= NpO2= 3.12502E-09 6.18962E-09 1.981 1.09008E-09 2.79779E-09 7.52738E-04
1957 NpO2OH(aq) NpO2OH(aq) 1.57050E-10 1.57050E-10 1.000 5.47828E-11 1.40605E-10 4.02206E-05
1958 H+ H+ 2.04048E-11 1.19335E-10 3.899 1.06757E-11 2.74002E-11 7.6166E-08
1959 NpO2(OH)2= NpO2(OH)2= 1.66773E-12 4.97826E-13 0.2985 5.81743E-13 1.49310E-12 4.53501E-07
1960 HCl(aq).....to.titrate.acid.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1961 NaOH(aq).....to.titrate.basess.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1962 NpO2OH(aq) NpO2OH(aq) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1963 NpO2OH(amor) NpO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1964 NaH2PO2(CO3)2(s)DISABLED_DISABLED 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1965 NaCl NaCl 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1966 NaHCO3 NaHCO3 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1967 Na2CO3.10H2O Na2CO3.10H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1968 Na2CO3.7H2O Na2CO3.7H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1969 Na2CO3.H2O Na2CO3.H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1970 Na3H(CO3)2.2H2O Na3H(CO3)2.2H2O 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1971
1972 pH (-log(aH+)); pOH(-log(aOH+)) 9.9232 10.5142
1973 Osmotic Coefficient= 1.240746
1974

```

Appendix N: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
1975 Equilibrium RH (h) = 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           *G/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:[SCRANS.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.

```

1 INPUT file name is:U1:[SCBASS.FMT.UH]NP_NACL_BM.IN:1
2 INGRESS file name is:U1:[SCBASS.FMT.UH]NP_NACL_BM.INGRESS:1
3 OUTPUT file name is:U1:[SCBASS.FMT.UH]NP_NACL_BM.OUT:2
4 CHENDAT file name is:U1:[SCBASS.FMT.UH]PWT_JOB_NP_NACL_TEST.CHENDAT:1
5 Temperature is Hard Coded as 298.15K
6 Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl          PWT V2.3
7 DATABASE: J0904/FW06; Np(V)-Na-CO3-OH-Cl-C1O4 (J0934);
8 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RPFR92,RPF94,RPFF94)
9
10 Accuracy of reactions is          1.000E-06
11 Minimum elemental abundance is    1.000E-18
12 Number of Aqueous Species is      50
13
14 Pitzer Data Base NOT Schoed in this Run
15
16 Species Order for Pitzer Parameters
17
18 Cations      13
19 Na+
20 MgB(OH)4+
21 K+
22 CaB(OH)4+
23 KpO3+
24
25 Anions      20
26 Cl-
27 B(OH)4-
28 ClO4-
29 HPO4-
30
31 Neutral     6
32 CO2(aq)
33 CaCO3(aq)
34 MgCO3(aq)
35 B(OH)3(aq)
36 HPO2OH(aq)
37 H3PO4(aq)
38
39 using Pitzer ACTIVITY COEFFICIENT model
40 Charge Balance replaces element Oxygen
41
42 this is a TITRATION problem
43
44 Ideal Gas Constant is Unity (Dimensionless)
45 Temperature = 298.15 [=] Degree Kelvin
46
47 115 Species      23 Elements
48
49 Element Name      Molecular Weight
50 Hydrogen           1.00790
51 Oxygen             15.99940
52 Sodium            22.98977
53 Potassium         39.09830
54 Magnesium         24.30500
55 Calcium          40.08000
56 Chlorine          35.45300
57 Sulfur            32.06000
58 Carbon            12.01100
59 Phosphorus        30.97400
60 Nitrogen          14.00640
61 Air               28.84000
62 Boron             10.81000
63 Bromine           79.90400
64 TracerEl         0.00000
65 Th(IV)            232.03810
66 Am(III)           243.00000
67 U(VI)             238.02900
68 Np(V)             237.04820
69 ClO4-(EL)        99.45060
70 Phosphorus       30.97400
71 Electron         0.00000
72 Charge           0.00000
73
74
75 Species Name      Phase      Mol.Wt.      Std Chemical Potential, u/RT
76 1 H2O              WATER     aqueous     18.015        -95.6635
77 2 Na+              Na+      aqueous     22.990        -105.6510
78 3 K+               K+       aqueous     39.098        -113.9570
79 4 Ca++             Ca++    aqueous     40.080        -223.3000
80 5 Mg++             Mg++    aqueous     24.305        -183.4680
81 6 MgOH+            MgOH+   aqueous     41.312        -251.9400
82 7 H+               H+      aqueous     1.008         0.0000
83 8 Cl-              Cl-     aqueous     35.453        -52.9550
84 9 SO4-             SO4-   aqueous     96.058        -300.3860
85 10 HSO4-            HSO4-  aqueous     97.066        -304.9420
86 11 OH-              OH-    aqueous     17.007        -63.4350
87 12 HCO3-            HCO3-  aqueous     61.017        -236.7510
88 13 CO3=             CO3=   aqueous     60.009        -212.9440
89 14 CO2(aq)          CO2(aq) aqueous     44.010        -155.6000
90 15 CaCO3(aq)        CaCO3(aq) aqueous     100.089       -443.5000
91 16 MgCO3(aq)        MgCO3(aq) aqueous     84.334        -403.1550
92 17 B(OH)3(aq)       B(OH)3(aq) aqueous     61.832        -390.8100
93 18 B(OH)4-          B(OH)4- aqueous     78.839        -465.2000
94 19 B(OH)3(OH)4-    B(OH)3(OH)4- aqueous     148.457       -963.7700
95 20 B(OH)2(OH)4-    B(OH)2(OH)4- aqueous     151.266       -1239.1000
96 21 CaB(OH)4+       CaB(OH)4+ aqueous     118.919       -592.3000
97 22 MgB(OH)4+       MgB(OH)4+ aqueous     103.144       -651.8900
98 23 Br-              Br-     aqueous     79.904        -399.9900
99 24 ClO4-            perchlorate ClO4- aqueous     99.451        -399.9900
100 25 NaOH(aq)         to.titrate.base.only aqueous     39.997        500.0000
101 26 HCl(aq)          to.titrate.acid.only aqueous     36.461        500.0000
102 27 HClO4(aq)       to.titrate.acid.only aqueous     100.459       500.0000
103 28 PosIon          POSITIVE ION aqueous     0.000         0.0000
104 29 NegIon          NEGATIVE ION aqueous     0.000         0.0000
105 30 PosIon(OH)(aq) to.titrate.base aqueous     17.007        500.0000
106 31 HNegIon(aq)     to.titrate.acid aqueous     1.008         500.0000
107 32 Tracer(aq)      conservative.tracer aqueous     0.000         0.0000
108 33 H3PO4(aq)       H3PO4(aq) aqueous     97.995        -460.9000
109 34 H2PO4-          H2PO4-  aqueous     96.987        -455.9600
110 35 HPO4=           HPO4=   aqueous     95.980        -439.1670
111 36 PO4=            PO4=    aqueous     94.972        -410.9470
112 37 HPO2+           HPO2+   aqueous     269.047       -369.1270
113 38 HPO2OH(aq)     HPO2OH(aq) aqueous     286.054       -438.5180
114 39 HPO2(OH)2-     HPO2(OH)2- aqueous     103.062       -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---	NpO2 (CO3) 3---	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	277.035	-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	Np2O7CO3 (s)	Np2O7CO3 (s)	solid	352.046	-713.7070
129	54	Np2O7 (CO3) 2 (s) DISABLED, O3 FAMILIAR		solid	458.025	-929.4900
130	55	AmOHC03 (c)	AmOHC03 (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	NaCl (SO4) 2 Aphthitalite	Aphthitalite	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	203.202	-853.1000
140	65	Na2Mg (SO4) 2. 4H2O	Bloedite	solid	334.461	-1383.6000
141	66	Mg (OH) 2	Burckite	solid	58.320	-335.4000
142	67	NaSO4 (SO4) 2	Burckite	solid	390.063	-1449.4000
143	68	CaCO3	Calcite	solid	100.089	-455.6000
144	69	CaCl2. 4H2O	CaCl2 Tetrahydrate	solid	183.047	-698.7000
145	70	Ca4Cl12 (OH) 6. 13H2O. CaOxychloride A		solid	567.467	-2658.4500
146	71	Ca2Cl12 (OH) 2. H2O. CaOxychloride B		solid	203.096	-778.4100
147	72	MgCl3. 6H2O	Carnallite	solid	277.854	-1020.3000
148	73	MgSO4. 7H2O	Epsomite	solid	246.469	-1157.8300
149	74	NaNa2 (CO3) 2. 5H2O	Gonyulsite	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	Hexahydrate	solid	228.454	-1061.6000
154	79	MgCl2SO4. 3H2O	Jainite	solid	248.960	-938.2000
155	80	KNO3	Kalinite	solid	100.115	-350.0600
156	81	MgSO4. H2O	Kieserite	solid	138.378	-579.8000
157	82	K2Mg (SO4) 2. 6H2O	Leonite	solid	366.678	-1403.9700
158	83	Na4Ca (SO4) 2. 2H2O	Lahille Salt	solid	456.242	-1751.4500
159	84	MgCO3	Magnesite	solid	84.314	-414.4500
160	85	MgCl (OH) 3. 4H2O	MgOxychloride	solid	207.146	-1029.6000
161	86	KNO3	Mercallite	solid	136.164	-417.5700
162	87	Na2SO4. 10H2O	Mirabilite	solid	322.189	-1471.1500
163	88	K8H6 (SO4) 7	Misenerite	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	Mesquehuite	solid	138.360	-695.3000
167	92	K2Mg (SO4) 2. 6H2O. Picromerite / Scheerite		solid	482.708	-159.1000
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	165.225	-577.3700
172	97	K8H4 (CO3) 6. 3H2O	R-Sequicarbonate	solid	730.919	-2555.4000
173	98	K2NaCO3. 6H2O	R-Na Carbonate	solid	219.188	-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	K3Ca (SO4) 2. H2O	Synymite	solid	338.407	-1164.8000
180	105	MgCl2Cl6. 12H2O	Tachyhydrite	solid	517.590	-2015.9000
181	106	Na2SO4	Thernardite	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	Boric Acid Solid	solid	61.832	-390.8800
186	111	K2B4O7. 4H2O	K-Pentaborate. (30_C)	solid	293.204	-1179.2600
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	Teepelite. (20_C)	solid	160.372	-725.7700

Truncated Name	Formula Matrix
194	1 H2O
195	2 Na+
196	3 K+
197	4 Ca++
198	5 Mg++
199	6 HPO4-
200	7 H+
201	8 Cl-
202	9 SO4-
203	10 HSO4-
204	11 OH-
205	12 HCO3-
206	13 CO3-
207	14 CO2 (aq)
208	15 CaCO3 (aq)
209	16 HgCO3 (aq)
210	17 B (OH) 3 (aq)
211	18 B (OH) 3
212	19 B3O3 (OH) 4-
213	20 B4O5 (OH) 4-
214	21 CaB (OH) 4+
215	22 HgB (OH) 4+
216	23 Br-
217	24 ClO4-
218	25 NaOH (aq) to. ti
219	26 HCl (aq) to. ti
220	27 HClO4 (aq) to. ti
221	28 PosIon
222	29 NegIon
223	30 PosIon (OH) (aq)
224	31 NegIon (aq) (aq)
225	32 Tracer (aq) cons
226	33 H3PO4 (aq)
227	34 H2PO4-
228	35 HPO4--
229	36 PO4--
230	37 NpO2+
231	38 NpO2OH (aq)
232	39 NpO2 (OH) 2-
233	40 NpO2CO3-
234	41 NpO2 (CO3) 2--
235	42 NpO2 (CO3) 3---
236	43 Am+++
237	44 AmCO3+
238	45 Am (CO3) 2-

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	8.57464E-01	8.59843E-01	1.003	5.55025E+01	5.00446E+01	9.01564E+05	
Na+	5.61052E+00	3.69881E+00	0.6593	5.61000E+00	5.05833E+00	1.16290E+05	
CO3-	1.99407E+00	4.9214E-02	2.0522E-02	1.99385E+00	1.79778E+00	1.07884E+05	
Cl-	1.61018E+00	1.06477E+00	0.6613	1.61000E+00	1.45168E+00	5.14664E+04	
HCO3-	6.14734E-03	1.59048E-03	0.2587	6.14665E-03	5.54222E-03	3.28170E+02	
OH-	6.14733E-03	4.86901E-03	0.7921	6.14665E-03	5.54221E-03	9.42580E+01	
CO2(aq)	2.36676E-09	7.15913E-09	3.022	2.36850E-09	2.13559E-09	3.39866E-05	2.07E-11
H+	2.39954E-12	1.77959E-12	0.7416	2.39927E-12	2.16334E-12	2.16043E-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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.30E+02
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.99E+01
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.51E+01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.63E+00
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.57E+00

384 pH (-log[mH+]); pOH(-log[mOH-]) 11.7497 11.6199
 385 Osmotic Coefficient= 0.908418
 386 Equilibrium RM (%) = 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 Total G/RT= -6.42133776E+03
 399
 400 Reaction # 1 sldsum 2.00000000000000
 401 This is a solid-only reaction
 402
 403 shifting left by 4.64434654478258
 404 calling maknumv for allomorphic reactions
 405 # inversions for batch plm 99
 406
 407 Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molar NaCl FMT V2.3
 408 DATABASE: IHW86/FWS6; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 409 95.01.31 Am(III)-Na-Cl-CO3-2M-PC4 (FWS85, FWS90, 991, RFFR2, RFF94, RFF94)
 410 Pressure= 1.00000E+00 [atm] Temperature= 2.98E+02 [K] Kelvin
 411
 412 Elemental Abundances for Plasm Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1.11018363E+02	1.11017591E+02	9.9383866E+01	1.0016902E+05	Hydrogen
1.05508682E+02	5.55113597E+01	4.96942389E+01	7.9507800E+05	Oxygen
1.56100000E+01	5.61057382E+00	5.02263116E+00	1.1549181E+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
5.6110000E+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	4.12839260E-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	Al3
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	1.30048121E+02	Np(IV)
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	-3.81809877E-15	0.00000000E+00	Charge

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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31822E-01	7.77959E-01	0.9352	5.55091E+01	4.96918E+01	8.95208E+05	
Na2NpO2CO3(s)	9.99932E+00	1.00000E+00	1.000	9.99939E+00	8.95147E+00	3.15133E+06	
Cl-	5.61096E+00	5.29329E+00	0.9434	5.61100E+00	5.02298E+00	1.78080E+05	
Na+	5.61057E+00	5.29268E+00	0.9433	5.61061E+00	5.02263E+00	1.15469E+05	
NpO2-	6.12705E-04	1.21978E-03	1.991	6.12709E-04	5.48499E-04	1.47572E+02	
CO2(aq)	3.86103E-04	1.12115E-03	2.904	3.86106E-04	3.45643E-04	1.52117E+01	
HCO3-	2.26571E-04	8.38810E-05	0.3702	2.26573E-04	2.02829E-04	1.23760E+01	1.23E-14
H+	1.21872E-06	4.78095E-06	3.923	1.21873E-06	1.09101E-06	1.09962E-02	1.23E-14
NpO2CO3-	1.33528E-07	2.42971E-07	1.820	1.33527E-07	1.19534E-07	1.93348E-02	1.85E-14
CO3-	3.09384E-08	8.03343E-09	2.5966E-02	3.09386E-08	2.76943E-08	1.64203E-03	0.00E+00
OH-	3.01685E-08	1.63977E-09	0.5435	3.01687E-08	2.70071E-09	4.59318E-05	1.23E-14
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--	1.98384E-11	5.13355E-16	2.5877E-05	1.98385E-11	1.77595E-11	6.90960E-06	0.00E+00
NpO2(OH)2-	2.04381E-16	6.10703E-17	0.2986	2.04383E-16	1.82964E-16	5.54494E-11	0.00E+00
NpO2(CO3)3--	1.35197E-16	9.87897E-26	7.8908E-10	1.35198E-16	1.20777E-16	5.03310E-11	-2.35E-09
HCl(aq).....to.titrate.acid.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+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(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+02
Na3H(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.02E+01
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.24E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.95E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.93E+00
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+00
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.36E+02
NpO2OH(aq)	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"

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467 pH (-log(aH+)); pmH(-log(mH+)) 5.3205 5.9141
486 Osmotic Coefficient= 1.241871
489 Equilibrium RM (#) = 77.795863
491 Ionic Strength (m) = 5.611188
492 Density, kg/m3 = 1188.93
493 fCO2(g); log(fCO2(g))= 3.400E-02 -1.47
494
495 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
496 - Gas "molality" and "activity" are gas partial pressures
497 - "Descriptor" means:
498 *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
499 *saturation index for minerals, SI=log10(IAP/Ksp)
500 *log10(activity) for aqueous species with very small concentrations
501 *log10(partial pressure) for gases
502
503 Total G/RT= -1.3332084E+04
504 Flashing Titration # 1
505 # inversions for batch pbm 17
506 Benchmark TITRATE Problem: Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
507 DATABASE: RHW84/FW85; Np(V)-Na-CO3-OH-Cl-C1O4 (RHW84)
508 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RRFP92,RRFP94)
509 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
510
511 Elemental Abundances for Flash Problem
512
513 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
514
515 3.85457174E+01 1.11017591E+02 9.93838868E+01 1.00169020E+05 Hydrogen
516 3.6707638E+01 5.55113597E+01 4.86942389E+01 7.95078006E+05 Oxygen
517 5.4254323E+00 5.61057382E+00 5.02263316E+00 1.15469181E+05 Sodium
518 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Potassium
519 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Magnesium
520 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Calcium
521 1.95016801E+00 5.61096998E+00 5.02297775E+00 1.78077910E+05 Chlorine
522 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Sulfur
523 3.47561578E+00 6.12839260E-04 5.48618892E-04 6.58946151E+00 Carbon
524 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Phosphorus
525 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Nitrogen
526 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Boron
527 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Bromine
528 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 TracerEl
529 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Th(IV)
530 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Am(III)
531 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 U(VI)
532 3.47561578E+00 6.12839260E-04 5.48618892E-04 1.30049121E+02 Np(V)
533 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 ClO4 (-EL)
534 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Phosphorus
535 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Electron
536 -1.94659251E-15 -5.6006736E-15 -5.01377045E-15 0.0000000E+00 Charge
537
538 Solution Parameters, Calculated
539 SOLUTION MASS 461.602144251003 grams
540 H2O MASS 347.563995068949 grams
541 TDS (g/kg) 328.106912108174 g/kgH2O
542
543 Specified Solution Density
544 DENSITY 1188.93254605458 kg/m3 = g/l
545
546 Solution Parameters Based on Specified Density
547 SOLUTION VOL 0.388249228926239 liters
548 TDS 293.724084133903 g/l
549
550 Density based on TDS and NaCl solutions 1188.93254605458 g/l
551 Percent relative error vs NaCl density 0.000000000000000E+00 %
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Appendix O: Sample Output File "Np_NaCl_BM.OUT"

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
611				
612				
613				
614	3.85957275E+01	1.11017746E+02	9.93891116E+01	1.00174286E+05 Hydrogen
615	3.66763098E+01	5.55107903E+01	4.96927232E+01	7.95110540E+05 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	1.95031182E+00	5.60931148E+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	6.18540120E-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	1.47561578E+00	1.72218651E-04	1.54179484E-04	1.65479691E+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	-1.36269746E-15	-3.91969811E-15	-3.50912649E-15	0.00000000E+00 Charge

Solution Parameters, Calculated
 SOLUTION MASS 461.465996173122 grams
 H2O MASS 347.653675849709 grams
 TDS(g/kg) 327.947988724245 g/kgH2O

Specified Solution Density
 DENSITY 1188.8511378691 kg/m³ = g/l

Solution Parameters Based on Specified Density
 SOLUTION VOL. 0.388329534508861 liters
 TDS 293.596828859294 g/l

Density based on TDS and NaCl solutions 1188.8511378691 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	
656								
657								
658								
659	H2O	WATER	8.31845E-01	7.78011E-01	0.9351	1.92978E+01	4.96944E+01	8.95254E+05
660	NaHPO2CO3(s)	NaHPO2CO3(s)	9.99718E+00	1.00000E+00	1.000	3.47556E+00	8.95002E+00	2.15082E+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-	3.82292E-09	2.46282E-09	0.5436	1.32878E-04	3.42177E-04	2.08707E+01
664	CO2(aq)	CO2(aq)	3.08476E-04	8.95671E-04	2.904	1.07243E-04	2.76165E-04	1.21539E+01
665	HPO2+	HPO2+	1.72065E-04	2.42481E-04	1.990	5.98258E-05	1.54059E-04	4.14492E+01
666	H+	H+	5.77346E-07	2.26410E-06	3.322	2.00716E-07	5.16872E-07	5.20955E-04
667	HPO2CO3-	HPO2CO3-	1.33573E-07	2.43010E-07	1.819	4.64370E-08	1.19581E-07	3.92490E-02
668	CO3=	CO3=	1.10196E-07	2.86188E-09	2.5971E-02	3.83099E-08	9.86531E-08	3.11E-10
669	OH-	OH-	3.82292E-09	2.46282E-09	0.5436	2.21466E-09	5.70303E-09	9.69322E-05
670	NpO2(OH)(aq)	NpO2(OH)(aq)	4.57851E-10	4.57851E-10	1.000	1.59174E-10	4.09893E-10	1.17252E-04
671	NpO2(CO3)2=	NpO2(CO3)2=	7.06677E-11	1.82925E-15	2.5885E-05	2.45679E-11	6.32656E-11	2.46144E+05
672	NpO2(CO3)3=	NpO2(CO3)3=	1.58546E-15	1.25405E-24	7.9097E-10	5.51192E-16	1.41939E-16	6.37413E-10
673	NpO2(OH)2-	NpO2(OH)2-	2.55901E-16	7.64679E-17	0.2988	8.89657E-17	2.29098E-16	6.94309E-11
674	HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
675	NaOH(aq).....to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
676	NpO2OH(aq)	NpO2OH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.988E+02
677	NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-1.14E+10
678	Na3HPO2(CO3)2(s)_DISABLED_DISABLED		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-9.16E+02
679	NaCl	Halite	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-1.23E+01
680	NaHCO3	NaHcolite	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-3.72E+00
681	Na2CO3.10H2O	Naatron	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-7.36E+00
682	Na2CO3.H2O	Na2CO3-Hepalysat	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-7.40E+00
683	Na2CO3.H2O	Thermonatrite	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	-7.69E+00
684	Na3H(CO3)2.2H2O	Trozo	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	+9.40E+00

685
 686 pH (-log(aH+)); pOH(-log(aOH+)) 5.6451 6.2386
 687 Osmotic Coefficient= 1.241740
 688 Equilibrium RH (%) = 77.802108
 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 *Og/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 Q/RT= -4.63438031E+03
 702 Flashing Titration # 1
 703 # inversions for batch pbm 28
 704 Benchmark TITRATE Problem; Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
 705 DATABASE: HSMH4/FMS8; Np(V)-Na-CO2-OH-Cl-ClO4 (HR94);
 706 95.01.31 Am(III)-Na-Cl-CO3-SO4-P04 (FRSR9; FRF90; P91; RFFR92; RFF94; RFF94)
 707 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
711				
712				
713	3.85999827E+01	1.11017943E+02	9.93906557E+01	1.00175842E+05 Hydrogen
714	3.66786674E+01	5.55109442E+01	4.96970938E+01	7.95123682E+05 Oxygen
715	5.42615709E+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	5.60950016E+00	5.02198092E+00	1.78044898E+05 Chlorine
720	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Sulfur
721	3.47582777E+00	7.90125217E-04	7.0737210E-04	8.49625462E+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	5.09865217E-05	4.56465295E-05	1.08204277E+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 O: Sample Output File "Np_NaCl_BM.OUT"

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735 -2.02795903E-15 -5.83264097E-15 -5.22176860E-15 0.00000000E+00 Charge
736
737
738 Solution Parameters, Calculated
739 SOLUTION MASS 461.701223994178 grams
740 H2O MASS 347.691387425364 grams
741 TDS(g/kg) 327.905265106076 g/kgH2O
742
743 Specified Solution Density
744 DENSITY 1188.82922080341 kg/m3 = g/l
745
746 Solution Parameters Based on Specified Density
747 SOLUTION VOL 0.388366315291810 liters
748 TDS 293.562629094818 g/l
749
750 Density based on TDS and NaCl solutions 1188.82922080341 g/l
751 Percent relative error vs NaCl density 0.00000000000000E+000 %
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31852E-01	7.78030E-01	0.9353	1.92999E+01	4.96952E+01	8.95267E+05	
NaHPO2CO3(s)	9.99622E+00	1.00000E+00	1.000	3.47560E+00	8.94928E+00	3.15056E+06	
Na+	5.61002E+00	5.29080E+00	0.9431	1.95056E+00	5.02247E+00	1.15465E+05	
Cl-	5.50950E+00	5.29073E+00	0.9432	1.95037E+00	5.02200E+00	1.78045E+05	
HCO3-	5.79854E-04	2.14495E-04	0.3703	2.01610E-04	5.19124E-04	3.18754E+01	
CO2(aq)	2.09764E-04	6.09047E-04	2.903	7.29332E-05	1.87795E-04	8.26481E+00	
HPO2+	5.08524E-05	1.01192E-04	1.990	1.76809E-05	4.55264E-05	1.22488E+01	-1.03E-10
CO3=	1.72976E-07	9.68700E-09	2.5972E-02	1.29680E-07	3.33913E-07	2.00378E-02	1.16E-10
H+	2.58815E-07	1.01481E-06	3.921	8.99877E-08	2.31708E-07	2.33539E-04	-1.00E-10
HPO2CO3-	1.33591E-07	2.43057E-07	1.819	4.64464E-08	1.19600E-07	3.93550E-02	4.94E-14
OH-	1.42122E-08	7.72597E-09	0.5435	4.94144E-09	1.27337E-08	2.16394E-04	1.02E-10
HPO2OH(aq)	1.01827E-10	1.01827E-10	1.000	1.04943E-10	2.70216E-10	7.72964E-05	-2.15E-11
HPO2(CO3)2=	2.29159E-10	6.19242E-15	2.5888E-05	8.31675E-11	2.14147E-10	8.33172E-05	1.24E-10
HPO2(CO3)3=	1.81536E-14	1.43695E-23	7.9155E-10	6.31186E-15	1.62523E-14	7.29851E-09	-3.61E-07
HPO2(OH)2-	3.74382E-16	1.12470E-16	0.2988	1.30865E-16	3.26962E-16	1.02120E-10	8.05E-11
HCl(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.45E+02
NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+02
HPO2OH(aged)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.79E+00
HPO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.39E+00
NaHPO2(CO3)2(s)_DISABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.35E+00
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.54E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.03E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.87E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.16E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.68E+00

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756 pH (-log(aH+)); pM(-log(mM+)) 5.9936 6.5870
757 Osmotic Coefficient = 1.241491
758 Equilibrium RH (%) = 77.803013
759 Ionic Strength (m) = 5.610081
760 Density, kg/m3 = 1188.83
761 fCO2(g); log(fCO2(g)) = 1.847E-02 -1.73
762
763 NOTES:
764 - Water "molality" is mole fraction H2O in aqueous phase
765 - Gas "molality" and "activity" are gas partial pressures
766 - "Descriptor" means:
767 *DG/RT/ln10 for species with nonzero concs. (convergence criterion)
768 *Saturation Index for minerals, SI=log10(IAP/Ksp)
769 *log10(activity) for aqueous species with very small concentrations
770 *log10(partial pressure) for gases
771
772 Total G/RT = -4.62462770E+03
773 Flashing Titration # 4
774 # inversions for batch pbm 25
775
776 I benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
777 DATABASE: IRRM84/PW86; Np(V)-Na-CO3-OH-Cl-O4 (RR94);
778 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRM89, FRP90, P91, RFR92, RFP94, RFP94)
779 Pressure = 1.00000E+00 (=) ATM Temperature = 2.98E+02 (=) Kelvin
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781 Elemental Abundances for Flash Problem
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31854E-01	7.78037E-01	0.9353	1.93007E+01	4.96952E+01	8.95269E+05	
NaHPO2CO3(s)	9.99580E+00	1.00000E+00	1.000	3.47561E+00	8.94893E+00	3.15044E+06	

```

859 Solution Parameters, Calculated
860 SOLUTION MASS 461.718525701536 grams
861 H2O MASS 347.706761264890 grams
862 TDS(g/kg) 327.896311310982 g/kgH2O
863
864 Specified Solution Density
865 DENSITY 1188.82463250872 kg/m3 = g/l
866
867 Solution Parameters Based on Specified Density
868 SOLUTION VOL 0.388182367824256 liters
869 TDS 293.555459469871 g/l
870
871 Density based on TDS and NaCl solutions 1188.82463250872 g/l
872 Percent relative error vs NaCl density 0.00000000000000E+000 %
873
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31854E-01	7.78037E-01	0.9353	1.93007E+01	4.96952E+01	8.95269E+05	
NaHPO2CO3(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"

859	Na+	Na+	5.61001E+00	5.29054E+00	0.9431	1.95064E+00	5.02247E+00	1.15465E+05
860	Cl-	Cl-	5.60933E+00	5.29050E+00	0.9432	1.95040E+00	5.02186E+00	1.78040E+05
861	HCO3-	HCO3-	7.06447E-04	2.61569E-04	0.3703	2.45636E-04	6.32460E-04	3.85909E+01
862	CO2(aq)	CO2(aq)	1.46506E-04	4.25377E-04	2.903	5.09412E-05	1.31162E-04	5.77243E+00
863	NpO2+	NpO2+	2.39307E-05	4.76176E-05	1.990	8.32007E-06	2.14344E-05	5.76418E+00
864	CO3=	CO3=	7.92644E-07	2.05869E-08	2.5972E-02	2.75608E-07	7.09630E-07	4.25843E-02
865	H+	H+	1.48381E-07	5.81763E-07	1.821	5.15932E-08	1.32841E-07	4.33891E-04
866	NpO2CO3-	NpO2CO3-	1.33598E-07	2.43049E-07	1.819	4.64539E-08	1.19605E-07	1.93572E-02
867	OH-	OH-	2.47909E-08	1.34770E-08	0.5436	8.41996E-09	2.21945E-08	3.77469E-04
868	NpO2(CO3)2=	NpO2(CO3)2=	5.08155E-10	1.31608E-14	2.5889E-05	1.76758E-10	4.55114E-10	1.77049E-04
869	NpO2OH(aq)	NpO2OH(aq)	2.47753E-10	2.47753E-10	1.000	8.61455E-11	2.21806E-10	6.34485E-05
870	NpO2(CO3)3=	NpO2(CO3)3=	8.19789E-14	6.49034E-23	7.9171E-10	2.85046E-14	7.13192E-14	3.29590E-08
871	NpO2(OH)2-	NpO2(OH)2-	5.28926E-16	1.61042E-16	0.2988	1.87388E-16	4.82483E-16	1.46222E-10
872	HCl(aq).....to titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
873	NaOH(aq).....to titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
874	NpO2OH(aq).....to titrate.base.only		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
875	NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
876	Na3NpO2(CO3)2(a) DISABLED		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
877	NaCl	NaClite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
878	NaHCO3	NaHcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
879	Na2CO3.10H2O	Na2con	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
880	Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
881	Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
882	NaH(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00

pH (-log(aH+)) = 6.2353 6.8286
 Osmotic Coefficient = 1.241856
 Equilibrium RN (%) = 77.803683
 Ionic strength (M) = 5.610034
 Density, kg/m3 = 1188.83
 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:
 *OJ/RZ/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/RZ = -4.63672945E+03
 Flashing Titration # 5
 # Inversions for batch phin 24
 Benchmark TITRATE Problem: Np(V)O2 with CO2 in 5.61molal NaCl
 DATABASE: NMR4/FMS4; Np(V)-Na-Cl-CO2-CO-Cl-CO4 (MR4) FMT V2.3
 95.01.31 Am(III)-Na-Cl-CO2-SO4-PO4 (FRGRS,FRF70,PS1,RTFR23,RTFR4,RTFR94)
 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	9.93917729E+01	1.00176565E+05	Hydrogen
3.66807466E+01	5.55114537E+01	4.96977765E+01	7.95134606E+05	Oxygen
5.42634673E+00	5.61000049E+00	5.02246891E+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	Positron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neutron
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	TracerZl
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	6.78667210E-04	6.05979363E-06	1.43646317E+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
-1.79306614E-15	-5.15657522E-15	-4.61653057E-15	0.00000000E+00	Charge

Solution Parameters, Calculated
 SOLUTION MASS 461.739961235951 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 0.00000000000000E+000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	0.31855E-01	7.78044E-01	0.9353	1.93017E+01	4.96953E+01	8.95271E+05	
Na3NpO2CO3(a)	0.00000E+00	1.00000E+00	1.000	3.47561E+00	8.94851E+00	3.15029E+04	
Na+	5.61000E+00	5.29021E+00	0.9430	1.95073E+00	5.02247E+00	1.15465E+05	
Cl-	5.60933E+00	5.29028E+00	0.9432	1.95043E+00	5.02186E+00	1.78034E+05	
HCO3-	8.74979E-04	2.3972E-04	0.3703	3.04252E-04	7.83343E-04	4.77973E+01	
CO2(aq)	6.22872E-05	1.80849E-04	2.903	2.16588E-05	5.57639E-05	2.45416E+00	
NpO2+	6.63303E-06	1.31976E-05	1.990	2.30647E-06	5.93836E-06	1.59770E+00	-4.41E-08
CO3=	2.8604E-06	7.42826E-08	2.5972E-02	9.34507E-07	2.56051E-06	1.53654E-01	-4.94E-08
NpO2CO3-	1.33506E-07	2.43083E-07	1.819	4.64540E-08	1.19613E-07	1.93595E-02	9.87E-13
OH-	7.22202E-08	3.92602E-08	0.5436	2.51127E-08	6.46566E-08	1.09963E-03	-5.99E-09
H+	5.09374E-08	1.99697E-07	1.920	1.77122E-08	4.56027E-08	4.59630E-05	5.87E-09
NpO2(CO3)2=	1.82431E-09	4.74903E-14	2.5890E-05	6.37833E-10	1.64220E-09	6.38924E-04	-3.56E-09
NpO2OH(aq)	2.00045E-10	2.00045E-10	1.000	6.95604E-11	1.79094E-10	5.12306E-05	7.57E-10
NpO2(CO3)3=	1.06720E-12	8.45057E-22	7.9184E-10	1.71892E-13	9.55434E-13	4.29018E-07	-1.27E-08
NpO2(OH)2-	1.26749E-15	7.78813E-16	0.2988	4.40807E-16	1.13493E-15	1.43953E-10	-4.84E-09
HCl(aq).....to titrate.acid.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.46E+02
NaOH(aq).....to titrate.base.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.97E+02
NpO2OH(aq).....to titrate.base.only	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.97E+00
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(a) DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.34E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E+01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.36E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.55E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.99E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.37E+00
NaH(CO3)2.2H2O	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"

983 pH (-log(aH+)); pmH(-log(mH+)) 6.6996 7.2930
984 Osmotic Coefficient= 1.241627
985 Equilibrium RH (%) = 77.804379
986 Ionic Strength (m) = 5.610010
987 Density, kg/m3 = 1188.82
988 fCO2(g); log(fCO2(g))= 5.484E-03 -2.26
989
990 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
991 - Gas "molality" and "activity" are gas partial pressures
992 - "Descriptor" means:
993 *GG/RT/ln10 for species with nonzero concs. (convergence criterion)
994 *Saturation Index for minerals, SI=log10(IAP/Ksp)
995 *log10(activity) for aqueous species with very small concentrations
996 *log10(partial pressure) for gases

998 Total G/RT= -4.63484576E+03
999 Flashing Titration # 6
1000 # inversions for batch pbm 20
1001 Benchmark TITRATE Problem: Np(V)O2 with CO2 in 5.61molal NaCl PWT V2.3
1002 DATABASE: IHW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1003 95.01.31 Am(III)-Na-Cl-CO3-PO4 (FRSR9, FRF90, P91, RFR92, RFP94, RFPF94)
1004 Pressure= 1.00000E+00 [-] ATM Temperature= 2.98E+02 [=] Kelvin
1005

1006 Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1.86006468E+01	1.11018357E+02	9.93915462E+01	1.00176739E+05	Hydrogen
3.66820272E+01	5.55118408E+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
1.95046381E+00	5.60897248E+00	5.02148052E+00	1.78025531E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47598202E+00	1.05368461E-03	9.4333564E-04	1.13703794E+01	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Positron
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Neutron
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	5.64774935E-07	4.51918500E-07	1.07124571E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4- (XL)
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

1034 Solution Parameters, Calculated
1035 SOLUTION MASS 461.76631602029 grams
1036 H2O MASS 347.744713769081 grams
1037 TDS(g/kg) 327.889016793691 g/kgH2O
1038
1039 Specified Solution Density
1040 DENSITY 1188.82089447700 kg/m3 = g/l
1041
1042 Solution Parameters Based on Specified Density
1043 SOLUTION VOL 0.388423847702623 liters
1044 TDS 293.549618457625 g/l
1045
1046 Density based on TDS and NaCl solutions 1188.82089447700 g/l
1047 Percent relative error vs NaCl solution 0.00000000000000E+000 %
1048
1049
1050

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31857E-01	7.78050E-01	0.9353	1.93029E+01	4.96953E+01	8.95271E+05	
NaH2PO4CO3(a)	9.99473E+00	1.00000E+00	1.000	3.47562E+00	8.94800E+00	3.15011E+06	
Na+	5.61000E+00	5.29000E+00	0.9430	1.95005E+00	5.02247E+00	1.15465E+05	
Cl-	5.60899E+00	5.28999E+00	0.9431	1.95046E+00	5.02148E+00	1.78027E+05	
HCO3-	9.92658E-04	3.67542E-04	0.3703	3.45192E-04	8.88699E-04	5.42258E+01	
CO3	5.67805E-05	1.47473E-06	2.5972E-03	1.97451E-05	5.08340E-05	1.05050E+00	
CO2(aq)	4.03803E-06	1.17243E-05	2.903	1.40420E-06	3.61513E-06	1.59101E-01	-4.23E-08
OH-	1.26379E-06	6.87070E-07	0.5437	4.39476E-07	1.13143E-06	1.92426E-02	-9.05E-08
NpO2+	3.34150E-07	6.64800E-07	1.990	1.16199E-07	2.99155E-07	8.04688E-02	1.77E-07
NpO2CO3-	1.33613E-07	2.43094E-07	1.819	4.64631E-08	1.19620E-07	3.93616E-02	3.39E-13
NpO2(CO3)2=	3.64151E-08	9.42826E-13	2.5892E-05	1.26632E-08	3.26014E-08	1.26841E-02	-1.13E-07
H+	2.91116E-08	1.14116E-08	3.920	1.01231E-09	2.60620E-09	3.62679E-08	1.24E-07
NpO2(CO3)3=	4.20537E-10	3.3083E-19	7.9204E-10	1.46239E-10	3.76494E-10	1.6974E-04	-2.13E-07
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-	1.95555E-14	5.84354E-15	0.2988	6.80031E-15	1.75074E-14	5.30581E-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(aqsd)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
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(a) DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.33E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E+01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.31E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.65E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.69E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.98E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.27E+00

1082 pH (-log(aH+)); pmH(-log(mH+)) 7.9427 8.5359
1083 Osmotic Coefficient= 1.281601
1084 Equilibrium RH (%) = 77.805007
1085 Ionic Strength (m) = 5.610057
1086 Density, kg/m3 = 1188.82
1087 fCO2(g); log(fCO2(g))= 3.555E-04 -3.45
1088
1089 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1090 - Gas "molality" and "activity" are gas partial pressures
1091 - "Descriptor" means:
1092 *GG/RT/ln10 for species with nonzero concs. (convergence criterion)
1093 *Saturation Index for minerals, SI=log10(IAP/Ksp)
1094 *log10(activity) for aqueous species with very small concentrations
1095 *log10(partial pressure) for gases

1098 Total G/RT= -4.63497996E+03
1099 Flashing Titration # 7
1100 # inversions for batch pbm 21
1101 Benchmark TITRATE Problem: Np(V)O2 with CO2 in 5.61molal NaCl PWT V2.3
1102 DATABASE: IHW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1103 95.01.31 Am(III)-Na-Cl-CO3-PO4 (FRSR9, FRF90, P91, RFR92, RFP94, RFPF94)
1104 Pressure= 1.00000E+00 [-] ATM Temperature= 2.98E+02 [=] Kelvin
1105
1106 Elemental Abundances for Flash Problem

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1107				
1108				
1109	3.86077395E+01	1.11018365E+02	9.93915827E+01	1.00176776E+05 Hydrogen
1110	3.68829651E+01	5.55121073E+01	4.96984096E+01	7.95144735E+05 Oxygen
1111	5.42654906E+00	5.61000051E+00	5.02247378E+00	1.15465517E+05 Sodium
1112	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Potassium
1113	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Magnesium
1114	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Calcium
1115	1.95048738E+00	5.60871794E+00	5.02132553E+00	1.78021054E+05 Chlorine
1116	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Sulfur
1117	3.47601251E+00	1.14118108E-03	1.02166873E-03	1.22712631E+01 Carbon
1118	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Position
1119	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Helium
1120	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Air
1121	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Boron
1122	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Bromine
1123	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 TracerK1
1124	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Th(IV)
1125	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Am(III)
1126	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 U(VI)
1127	3.47561578E+00	3.61660997E-07	3.23784797E-07	7.67526032E-02 Np(V)
1128	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 ClO4-(EL)
1129	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Phosphorus
1130	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Electron
1131	-1.71147437E-15	-4.92142480E-15	-4.80601154E-15	0.00000000E+00 Charge

Solution Parameters, Calculated
 SOLUTION MASS 461.786282369672 grams
 H2O MASS 347.759934523067 grams
 TDS (g/kg) 327.888110522674 g/kgH2O

Specified Solution Density 1188.82043006313 kg/m³ = g/l
 DENSITY

Solution Parameters Based on Specified Density
 SOLUTION VOL 0.388440735614523 liters
 TDS 293.548892768997 g/l

Density based on TDS and NaCl solutions 1188.82043006313 g/l
 Percent relative error vs NaCl density 0.00000000000000000000 %

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
1154	H2O	8.31858E-01	7.78054E-01	0.9353	1.93037E+01	4.86953E+01	8.95272E+05
1155	NaHPO2CO3(s)	9.99430E+00	1.00000E+00	1.000	3.47562E+00	8.84761E+00	3.14997E+06
1156	Na+	5.61000E+00	5.28994E+00	0.9429	1.95093E+00	5.02247E+00	1.15466E+05
1157	Cl-	5.60872E+00	5.28973E+00	0.9431	1.95049E+00	5.02133E+00	1.78021E+05
1158	HCO3-	9.99205E-04	3.69908E-04	0.3703	3.47488E-04	6.94560E-04	5.45835E+01
1159	CO3=	1.39997E-04	3.63604E-06	2.5972E-02	4.86855E-05	1.25336E-04	7.52130E+00
1160	OH-	3.09556E-06	1.68295E-06	0.5437	1.07651E-06	2.77137E-06	4.71335E-02
1161	CO2(aq)	1.65938E-06	4.81799E-06	2.903	5.77065E-07	1.48559E-06	6.53807E-02
1162	NpO2+	1.35537E-07	2.89637E-07	1.989	4.71342E-08	1.21342E-07	3.26468E-02
1163	NpO2CO3-	1.33616E-07	2.43097E-07	1.619	4.64663E-08	1.19623E-07	3.93620E-02
1164	NpO2(CO3)2=	8.77711E-12	2.32472E-12	2.5894E-05	3.12209E-08	8.03749E-08	3.12711E-02
1165	NpO2(CO3)3=	2.55580E-09	2.02485E-18	7.9225E-10	8.88807E-10	2.28814E-09	1.02755E-03
1166	H+	1.18855E-09	4.65884E-09	3.920	4.13329E-10	1.06407E-09	1.07248E-06
1167	NpO2OH(aq)	1.75190E-10	1.75190E-10	1.000	6.09240E-11	1.56842E-10	4.48655E-05
1168	NpO2(OH)2-	4.75887E-14	1.42202E-14	0.2988	1.65494E-14	4.26048E-14	1.29119E-08
1169	HCl(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1170	NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1171	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1172	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1173	Na3NpO2(CO3)2(s)_DISABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1174	NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1175	NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1176	Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1177	Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1178	Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
1179	Na3H(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00

1181 pH (-log(aH+)); pOH(-log(aOH+)) 8.3317 8.9250
 1182 Osmotic Coefficient= 1.241589
 1183 Equilibrium RH (s) = 77.80533
 1184 Ionic Strength (m) = 5.610141
 1185 Density, kg/m³ = 1188.82
 1186 fCO2(g); log(fCO2(g)) = 1.461E-04 -1.84

1187 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
 1188 Gas "molality" and "activity" are gas partial pressures
 1189 - "Descriptor" means:
 1190 *dg/RT*ln10 for species with nonzero concs. (convergence criterion)
 1191 *saturation index for minerals, SI=log10(IAP/Ksp)
 1192 *log10(activity) for aqueous species with very small concentrations
 1193 *log10(partial pressure) for gases

1194
 1195 Total G/RT= -4.63507818E+03
 1196 Flashing Titration # 8
 1197 # inversions for batch pbim 21
 1198
 1199 benchmark TITRATE Problem: Np(V)O2 with CO2 in 5.61molal NaCl FMT V2.3
 1200 DATABASE: NMR84/PWR8; Np(V)-Na-CO3-OH-Cl-ClO4 (MR94);
 1201 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRMR9, FRP9, RFFR92, RFFR94, RFFR94)
 1202 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
 1203

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
1207				
1208	3.86097415E+01	1.11018371E+02	9.93916217E+01	1.00176815E+05 Hydrogen
1209	3.68840743E+01	5.55124212E+01	4.96987076E+01	7.95149502E+05 Oxygen
1210	5.42665021E+00	5.61000082E+00	5.02247577E+00	1.15465563E+05 Sodium
1211	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Potassium
1212	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Magnesium
1213	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Calcium
1214	1.95051642E+00	5.60851089E+00	5.02114187E+00	1.78014543E+05 Chlorine
1215	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Sulfur
1216	3.47604858E+00	1.14484251E-03	1.11447244E-03	1.33859285E+01 Carbon
1217	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Position
1218	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Helium
1219	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Air
1220	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Boron
1221	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Bromine
1222	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 TracerK1
1223	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Th(IV)
1224	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Am(III)
1225	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 U(VI)
1226	3.47561578E+00	3.74514610E-07	3.35282385E-07	7.94804563E-02 Np(V)
1227	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 ClO4-(EL)
1228	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Phosphorus
1229	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00 Electron
1230	-1.31010731E-15	-3.76707986E-15	-3.37256052E-15	0.00000000E+00 Charge

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```

1231 Solution Parameters, Calculated
1232 SOLUTION MASS 461.809836667171 grams
1233 H2O MASS 347.777949659092 grams
1234 TDS (g/kg) 327.887052988433 g/kgH2O
1235
1236 Specified Solution Density
1237 DENSITY 1188.81988813375 kg/m^3 = g/l
1238
1239 Solution Parameters Based on Specified Density
1240 SOLUTION VOL 0.388460725864989 liters
1241 TDS 293.548045955388 g/l
1242
1243 Density based on TDS and NaCl solutions 1188.81988813375 g/l
1244 Percent relative error vs NaCl density 0.000000000000000000 %
1245
1246
1247
1248
1249
1250

```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31859E-01	7.78058E-01	0.9353	1.93047E+01	4.96954E+01	8.95272E+05	
NaHPO2CO3(s)	9.99378E+00	1.00000E+00	1.000	3.47562E+00	8.94715E+00	3.14981E+06	
Na+	5.61000E+00	5.28987E+00	0.9429	1.95103E+00	5.02248E+00	1.15466E+05	
Cl-	5.60851E+00	5.28943E+00	0.9431	1.95052E+00	5.02114E+00	1.78015E+05	
HCO3-	1.00274E-03	3.71260E-04	0.3702	3.48729E-04	8.97721E-04	5.47764E+01	
CO3=	2.40670E-04	6.25064E-06	2.5972E-02	8.36995E-05	2.15465E-04	1.29299E+01	
OH-	5.30281E-06	2.80301E-06	0.5437	1.84420E-06	4.74746E-06	8.07415E-02	-2.63E-07
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=	1.54320E-07	3.99643E-12	2.5897E-05	5.26690E-08	1.38158E-07	5.37525E-02	1.94E-08
NpO2CO3-	1.33620E-07	2.43100E-07	1.819	4.64701E-08	1.19626E-07	3.93638E-02	1.72E-11
NpO2+	7.88495E-08	1.56851E-07	1.989	2.74221E-08	7.05917E-08	1.89925E-02	-1.38E-08
NpO2(CO3)3=	7.55070E-09	5.98397E-18	7.9251E-10	2.62597E-09	6.75993E-09	3.03571E-03	1.34E-08
H+	6.93877E-10	2.71860E-09	3.919	2.43115E-10	6.21208E-10	5.26116E-07	2.77E-08
NpO2OH(aq)	1.74579E-10	1.74579E-10	1.000	6.07149E-11	1.56296E-10	4.47092E-05	-1.42E-08
NpO2(OH)2-	8.12402E-14	2.42753E-14	0.2988	2.82535E-14	7.27320E-14	2.20423E-08	-6.38E-08
HCl(aq).....to.titrant.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.titrant.basess.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
NpO2OH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
NpO2OH(amor)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.62E+00
Na3NpO2(CO3)2(s)_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.32E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E+01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.02E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.06E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.35E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.64E+00

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1280 pH (-log(aH+)), pOH(-log(aOH+)) 8.5655 9.1587
1281 Osmotic Coefficient= 1.241574
1282 Equilibrium RN (R) = 77.805756
1283 Ionic Strength (m) = 5.610242
1284 Density, kg/m3 = 1188.82
1285 fCO2(g); log(fCO2(g))= 8.559E-05 -4.07
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= -4.6318432E+03
1296 Flashing Titration # 9
1297 # inversions for batch pbm 22
1298
1299 Benchmark TITRATE Problem: Np(V)O2 with CO3 in 5.61molal NaCl
1300 DATABASE: HEN84/FM86; Np(V)-Na-CO3-OH-Cl-C1O4 (NR94);
1301 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (PKSR89,PKFP90,PKFP91,PKFP92,PKFP94,PKFP94)
1302 Pressure= 1.00000E+00 [atm] Temperature= 2.98E+02 [K] Kelvin
1303
1304 Elemental Abundances for Flash Problem
1305
1306 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
1307 1.46117435E+01 1.11018376E+02 9.93916598E+01 1.00176854E+05 Hydrogen
1308 3.66851835E+01 5.55127148E+01 4.96990052E+01 7.95154264E+05 Oxygen
1309 5.42675140E+00 5.61000112E+00 5.02247774E+00 1.15465608E+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 1.9505219E+00 5.6083381E+00 5.0215819E+00 1.78009312E+05 Chlorine
1314 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1315 3.47608464E+00 1.34852749E+01 1.20729910E+01 4.05008694E+01 Carbon
1316 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 PotIion
1317 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 NaqIon
1318 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Alr
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 4.23659533E-07 3.7929532E-07 8.99122713E-02 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 -1.32066722E-15 -3.79724708E-15 -3.39956948E-15 0.00000000E+00 Charge
1330
1331 Solution Parameters, Calculated
1332 SOLUTION MASS 461.833395409572 grams
1333 H2O MASS 347.795967232738 grams
1334 TDS (g/kg) 327.885998692483 g/kgH2O
1335
1336 Specified Solution Density
1337 DENSITY 1188.81934786396 kg/m^3 = g/l
1338
1339 Solution Parameters Based on Specified Density
1340 SOLUTION VOL 0.388460719328282 liters
1341 TDS 293.547201735043 g/l
1342
1343 Density based on TDS and NaCl solutions 1188.81934786396 g/l
1344 Percent relative error vs NaCl density 0.000000000000000000 %
1345
1346
1347
1348
1349
1350

```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31861E-01	7.78062E-01	0.9353	1.93057E+01	4.96954E+01	8.95272E+05	
NaHPO2CO3(s)	9.99326E+00	1.00000E+00	1.000	3.47562E+00	8.94669E+00	3.14981E+06	
Na+	5.61000E+00	5.28981E+00	0.9429	1.95114E+00	5.02248E+00	1.15466E+05	

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

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1355 Cl- Cl- 5.60830E+00 5.28912E+00 0.9411 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- 7.50944E-06 4.08299E-06 0.5437 2.61189E-06 6.72335E-06 1.14346E-01
1359 CO2(aq) CO2(aq) 6.88224E-07 1.99826E-06 2.904 2.19361E-07 6.16147E-07 2.71165E-02
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
1361 NpO2CO3- NpO2CO3- 1.33624E-07 2.43103E-07 1.819 4.64739E-08 1.19630E-07 3.33649E-02
1362 NpO2+ NpO2+ 5.55313E-08 1.10457E-07 1.989 1.93136E-08 4.97156E-08 1.33758E-02
1363 NpO2(CO3)3= NpO2(CO3)3= 1.52213E-08 1.20666E-17 7.9276E-10 5.29390E-09 1.36272E-08 6.11963E-03
1364 H+ H+ 4.89995E-10 1.92033E-09 3.919 1.70418E-10 4.38679E-10 4.42145E-07
1365 NpO2OH(aq) NpO2OH(aq) 1.74113E-10 1.74113E-10 1.000 6.0558E-11 1.55879E-10 4.45898E-05
1366 NpO2(OH)2- NpO2(OH)2- 1.14749E-13 3.42875E-14 0.2988 3.99952E-14 1.02731E-13 3.11393E-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
1368 NaOH(aq).....to.titrate.base.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1369 NpO2OH(aged) NpO2OH(aged) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1370 NpO2OH(amor) NpO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+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
1372 NaCl NaClite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1373 NaHCO3 NaHcolite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1374 Na2CO3.10H2O Naatron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1375 Na2CO3.7H2O Na2CO3-Heptahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1376 Na2CO3.H2O Thermonatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1377 NaH(CO3)2.2H2O Trona 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1378
1379 pH (-log[AH+]); pOH(-log[OH-]) 8.7166 9.3098
1380 Osmotic Coefficient= 1.241560
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 *G/R/T/ln10 for species with nonzero concs. (convergence criterion)
1390 *Saturation Index for minerals, SI=log(IAP/Ksp)
1391 *log10(activity) for aqueous species with very small concentrations
1392 *log10(partial pressure) for gases
1393
1394 Total G/R/T= -4.63531045E+03
1395 Flashing Titration # 10
1396 # iterations for batch phm 22
1397 Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl PWT V2.3
1398 DATABASE: NPH84/PW86; Np(V)-Na-CO3-OM-Cl-ClO4 (NR94);
1399 95.01.31 Am(III)-Na-Cl-CO3-SD4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRF94)
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 3.86146895E+01 1.11018381E+02 9.93917155E+01 1.00176910E+05 Hydrogen
1407 3.86868157E+01 5.55131962E+01 4.96994412E+01 7.95161269E+05 Oxygen
1408 5.42490038E+00 5.61000158E+00 5.02248060E+00 1.15446750E+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 3.4761372E+00 1.50110283E-03 1.34389622E-03 6.61815176E+01 Carbon
1415 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1416 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Nitrogen
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 Tellurium
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 4.64118535E-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 461.8680648466891 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/m3 = g/l
1437
1438 Solution Parameters Based on Specified Density
1439 SOLUTION VOL 0.388514115444 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+00 %
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 8.31842E-01 7.78067E-01 0.9353 1.93072E+01 4.96954E+01 8.95273E+05
1452 NaNpO2CO3(s) NaNpO2CO3(s) 9.99250E+00 1.00000E+00 1.000 3.47542E+00 8.94601E+00 3.14841E+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 5.28672E+00 0.9431 1.95059E+00 5.02069E+00 1.77998E+05
1455 HCO3- HCO3- 1.00903E-03 3.75727E-04 0.3702 3.50963E-04 9.03156E-04 5.51202E+01
1456 CO3= CO3= 4.90734E-04 1.27449E-05 2.5971E-02 1.70688E-04 4.39341E-04 2.63845E+01
1457 OH- OH- 0.74513E-05 5.84210E-06 0.5437 3.73739E-06 9.61980E-06 1.63607E-01
1458 CO2(aq) CO2(aq) 4.82685E-07 1.40148E-06 2.904 1.67889E-07 4.32135E-07 1.90182E-02
1459 NpO2(CO3)2= NpO2(CO3)2= 3.14582E-07 8.14888E-12 2.5904E-05 1.09419E-07 2.81617E-07 1.09575E-01
1460 NpO2CO3- NpO2CO3- 1.33630E-07 2.43107E-07 1.819 4.64794E-08 1.19635E-07 3.33668E-02
1461 NpO2+ NpO2+ 3.86794E-08 7.69287E-08 1.989 1.34536E-08 3.46286E-08 9.31671E-03
1462 NpO2(CO3)3= NpO2(CO3)3= 3.13678E-08 2.48787E-17 7.9313E-10 1.09104E-08 2.80827E-08 1.26112E-02
1463 H+ H+ 4.89995E-10 1.92033E-09 3.919 1.70418E-10 4.38679E-10 4.466E-08
1464 NpO2OH(aq) NpO2OH(aq) 1.73507E-10 1.73507E-10 1.000 6.03495E-11 1.55336E-10 4.44344E-05
1465 NpO2(OH)2- NpO2(OH)2- 1.63619E-13 4.88895E-14 0.2988 5.69105E-14 1.46484E-13 4.43936E-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
1467 NaOH(aq).....to.titrate.base.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1468 NpO2OH(aged) NpO2OH(aged) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1469 NpO2OH(amor) NpO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+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
1471 NaCl NaClite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1472 NaHCO3 NaHcolite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1473 Na2CO3.10H2O Naatron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1474 Na2CO3.7H2O Na2CO3-Heptahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1475 Na2CO3.H2O Thermonatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1476 NaH(CO3)2.2H2O Trona 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1477
1478 pH (-log[AH+]); pOH(-log[OH-]) 8.8722 9.4653

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Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
1479 Osmotic Coefficient= 1.241539
1480 Equilibrium RH (%) = 77.802748
1481 Ionic Strength (m) = 5.610494
1482 Density, kg/m3 = 1188.82
1483 fCO2(g); log(fCO2(g))= 4.250E-05 -4.37
1484
1485 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1486 - Gas "molality" and "activity" are gas partial pressures
1487 - "Descriptor" means:
1488 *dg/RT/ln10 for species with nonzero concs. (convergence criterion)
1489 *Saturation Index for minerals, SI=log10(IAP/Ksp)
1490 *log10(activity) for aqueous species with very small concentrations
1491 *log10(partial pressure) for gases
1492
1493 Total Q/RT= -4.63548130E+03
1494 Flashing Titration # 11
1495 # inversions for batch pbm 23
1496 Benchmark TITRATE Problem: Np(V)O2 with CO2 in 5.61molal NaCl PWT V2.3
1497 DATABASE: HMR84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1498 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFPF92,RFPF94)
1499 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1500
```

1501 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
1.6593889E+01	5.5515218E+01	4.9701271E+01	7.95190533E+05	Oxygen
5.42752259E+00	5.61000344E+00	5.0224827E+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
1.47635958E+00	2.11879271E+03	1.9148054E+03	2.29897401E+01	Carbon
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	Nitrogen
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	Titanium
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

1529 Solution Parameters, Calculated

SOLUTION MASS	462.013011582888	grams
H2O MASS	297.93328203232	grams
TDS (g/kg)	127.877998835092	g/kgH2O

1534 Specified Solution Density

DENSITY	1188.81524835729	kg/m ³ = g/l
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1537 Solution Parameters Based on Specified Density

SOLUTION VOL	0.388633147348740	liters
TDS	293.540795885520	g/l

1541 Density based on TDS and NaCl solutions 1188.81524835729 g/l

1542 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	8.31870E-01	7.78092E-01	0.9354	1.93133E+01	4.96955E+01	8.95274E+05	
NaHPO2CO3(a)	9.98931E+00	1.00000E+00	1.000	1.47562E+00	8.94318E+00	1.14841E+06	
Na+	5.61000E+00	5.28932E+00	0.9428	1.95191E+00	5.02249E+00	1.15466E+05	
Cl-	5.60673E+00	5.28679E+00	0.9429	1.95077E+00	5.01956E+00	1.77958E+05	
CO3=	1.11397E-03	2.89290E-05	2.5969E-02	3.87586E-04	9.97306E-04	5.98475E+01	
HCO3-	1.02256E-03	3.78536E-04	0.3702	3.55788E-04	9.15475E-04	5.58596E+01	
OH-	2.40681E-05	1.30872E-05	0.5438	8.37409E-06	2.15475E-05	1.68485E-01	-4.77E-09
NpO2(CO3)2=	7.13640E-07	1.84981E-11	1.5921E-05	2.48299E-07	6.38904E-07	2.48575E-01	9.86E-09
CO2(aq)	2.18331E-07	6.3194E-07	2.904	7.59645E-08	1.95466E-07	8.60242E-03	-1.95E-08
NpO2(CO3)3=	1.61308E-07	1.28190E-16	7.9469E-10	5.61244E-08	1.44415E-07	6.48530E-02	1.95E-08
NpO2CO3-	1.33654E-07	2.43125E-07	1.819	4.65026E-08	1.19657E-07	3.93738E-02	1.59E-12
NpO2+	1.70496E-08	3.38942E-08	1.988	5.93214E-09	1.52641E-08	4.10676E-03	-9.06E-09
NpO2OH(aq)	1.71249E-10	1.71249E-10	1.000	5.95834E-11	1.53135E-10	4.38545E-05	1.05E-08
H+	1.59918E-10	5.99136E-10	1.916	5.32272E-11	1.36908E-10	1.8042E-07	-1.95E-08
NpO2(OH)2-	3.61801E-13	1.08049E-13	0.2988	1.25883E-13	3.23912E-13	9.61651E-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)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.04E+00
NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.63E+00
NaHPO2(CO3)2(s) DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.32E+02
NaCl	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.24E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.30E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.36E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.39E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.48E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.96E+00

```
1577 pH (-log(aH+)); pmf(-log(mf+)) 9.2225 9.8154
1578 Osmotic Coefficient= 1.241451
1579 Equilibrium RH (%) = 77.809217
1580 Ionic Strength (m) = 5.611321
1581 Density, kg/m3 = 1188.82
1582 fCO2(g); log(fCO2(g))= 1.922E-05 -4.72
1583
1584 NOTES: - Water "molality" is mole fraction H2O in aqueous phase
1585 - Gas "molality" and "activity" are gas partial pressures
1586 - "Descriptor" means:
1587 *dg/RT/ln10 for species with nonzero concs. (convergence criterion)
1588 *Saturation Index for minerals, SI=log10(IAP/Ksp)
1589 *log10(activity) for aqueous species with very small concentrations
1590 *log10(partial pressure) for gases
1591
1592 Total Q/RT= -4.63619543E+03
1593 Flashing Titration # 12
1594 # inversions for batch pbm 23
1595 Benchmark TITRATE Problem: Np(V)O2 with CO2 in 5.61molal NaCl PWT V2.3
1596 DATABASE: HMR84/FM86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1597 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFPF92,RFPF94)
1598 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin
1599
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1600 Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
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Appendix O: Sample Output File "Np_NaCl_BM.OUT"

1603	1.86445564E+01	1.11018446E+02	9.93922712E+01	1.00177470E+05	Hydrogen
1604	3.67032632E+01	5.55178691E+01	4.97018762E+01	7.95232196E+05	Oxygen
1605	5.4284952E+00	5.61000623E+00	5.02251004E+00	1.15466353E+05	Sodium
1606	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Potassium
1607	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Magnesium
1608	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Calcium
1609	1.95102113E+00	5.60491244E+00	5.01794862E+00	1.77901170E+05	Chlorine
1610	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
1611	3.47667577E+00	3.04710993E-03	2.72800770E-03	3.27661005E+01	Carbon
1612	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon
1613	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon
1614	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Alr
1615	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Boron
1616	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Bromine
1617	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	TracerEl
1618	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Th(IV)
1619	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Am(III)
1620	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(VI)
1621	3.47561578E+00	1.94420912E-06	1.74050000E-06	4.13607419E-01	Np(VI)
1622	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4-(EL)
1623	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
1624	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron
1625	-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/m³ = g/l
Solution Parameters Based on Specified Density
SOLUTION VOL. 0.388808464732340 liters
TDS 293.533478748712 g/l
Density based on TDS and NaCl solutions 1188.81056566046 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	8.31881E-01	7.78127E-01	0.9354	1.93221E+01	4.96957E+01	8.95277E+05
NaHPO4(CO3)(s)	NaHPO4(CO3)(s)	9.98478E+00	1.00000E+00	1.000	3.47562E+00	8.93914E+00	1.14699E+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=	2.00200E-03	5.19855E-05	2.5967E-02	6.88800E-04	1.79215E-03	1.07557E+02
HCO3-	HCO3-	1.94073E-03	1.85192E-05	0.3701	1.62267E-04	9.1738E-04	5.68519E+01
OH-	OH-	4.24987E-05	2.11124E-05	0.5438	1.47934E-05	3.80481E-05	6.47095E-01
NpO2(CO3)2=	NpO2(CO3)2=	1.26136E-06	3.2444E-11	2.5945E-05	4.46030E-07	1.14717E-06	4.46325E-01
NpO2(CO3)3=	NpO2(CO3)3=	5.19497E-07	4.13996E-16	7.9692E-10	1.80832E-07	4.65094E-07	2.08662E-01
NpO2CO3-	NpO2CO3-	1.23688E-07	2.43151E-07	1.819	4.65356E-08	1.19688E-07	3.93840E-02
CO2(aq)	CO2(aq)	1.25795E-07	3.62721E-07	2.904	4.37896E-08	1.12625E-07	4.95661E-03
NpO2	NpO2	9.49502E-09	8.8635E-08	1.987	1.10513E-09	8.50067E-09	2.28708E-01
NpO2OH(aq)	NpO2OH(aq)	1.68316E-10	1.68316E-10	1.000	5.85892E-11	1.50689E-10	4.31052E-05
H+	H+	8.66958E-11	3.29270E-10	3.913	3.01780E-11	7.76167E-11	7.82299E-08
NpO2(OH)2-	NpO2(OH)2-	6.28103E-13	1.87627E-13	0.2987	2.18637E-13	5.62326E-13	1.70419E-07
HCl(aq).....to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	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	-2.94E+02
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-1.05E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-3.64E+00
Na3NpO2(CO3)2(s)_DISABLED		0.00000E+00	1.00000E+00	1.000	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	-1.24E+01
NaNCO3	NaHcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.29E+00
Na2CO3.10H2O	Naatron	0.00000E+00	1.00000E+00	1.000	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	-1.14E+00
Na2CO3	Thermonatrite	0.00000E+00	1.00000E+00	1.000	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	-4.70E+00

pH (-log(aH+)); pOH(-log(aOH)) 9.4695 10.0620
Osmotic Coefficient= 1.241325
Equilibrium RH (%) = 77.812731
Ionic Strength (m) = 5.612017
Density, kg/m³ = 1188.81
fCO2(g); logfCO2(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:
*dq/dT/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 Q/RT= -4.63721297E+03
Flashing Titration # 13
Inversions for batch plm 29
Benchmark TITRATE Problem: Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.3
DATABASE: IGM84/FWS6; Np(V)-Na-CO3-OH-Cl-ClO4 (HR94);
95.01.31 Am(III)-Na-Cl-CO3-FO4 (FRS89,FRF90,PF1,RRFR92,RRF94,RRF94)
Pressure= 1.0000E+00 (=) ATM Temperature= 2.985E+02 (=) Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
3.87052172E+01	1.11018564E+02	9.93931710E+01	1.00178579E+05	Hydrogen
1.67369721E+01	5.55273415E+01	4.97128540E+01	7.95175837E+05	Oxygen
5.43147487E+00	5.61001896E+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	5.60495735E+00	5.01239802E+00	1.77704610E+05	Chlorine
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Sulfur
3.47776859E+00	4.18159604E-03	5.53429668E-03	6.44724375E+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	Alr
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	6.65371933E-06	5.96591485E-06	1.41421432E+00	Np(VI)
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
-1.62237641E-15	-4.65347858E-15	-4.16619444E-15	0.00000000E+00	Charge

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```

1727 Solution Parameters, Calculated
1728 SOLUTION MASS 462.933837982393 grams
1729 H2O MASS 348.637344066918 grams
1730 TDS(g/kg) 327.837782901256 g/kgH2O
1731
1732 Specified Solution Density
1733 DENSITY 1188.79463948067 kg/m3 = g/l
1734
1735 Solution Parameters Based on Specified Density
1736 SOLUTION VOL 0.389414472952726 liters
1737 TDS 293.508592654065 g/l
1738
1739 Density based on TDS and NaCl solutions 1188.79463948067 g/l
1740 Percent relative error vs NaCl density 0.000000000000000000 %
1741
1742
1743
1744

```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.31919E-01	7.78249E-01	0.9355	1.93524E+01	4.96991E+01	8.95286E+05	
NaH2PO4(aq)	9.96914E+00	1.00000E+00	1.000	3.47561E+00	8.92523E+00	3.14209E+06	
Na+	5.61002E+00	5.28890E+00	0.9424	1.95586E+00	5.02257E+00	1.15468E+05	
Cl-	5.59866E+00	5.27483E+00	0.9422	1.95190E+00	5.01240E+00	1.77705E+05	
CO3=	5.06639E-03	1.31512E-04	2.5957E-02	1.76633E-03	4.53587E-03	2.72194E+02	
HCO3-	1.09876E-03	4.06390E-04	0.3699	3.82038E-04	9.81625E-04	4.00180E+01	
OH-	1.01868E-04	5.54275E-05	0.5441	3.55148E-05	9.12006E-05	1.55108E+00	-1.56E-10
NpO2(CO3)2=	3.29369E-06	2.65037E-15	8.0468E-10	1.14803E-06	2.94880E-06	1.22422E+00	1.74E-09
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-	1.33806E-07	2.43237E-07	1.818	4.66498E-08	1.19795E-07	3.94192E-02	5.06E-13
CO2(aq)	5.53195E-08	1.60694E-07	2.904	1.92934E-08	4.95446E-08	2.18045E-03	-9.19E-09
NpO2=	3.76315E-09	7.45927E-09	1.982	1.31197E-09	3.36909E-09	9.06445E-04	-7.94E-10
NpO2OH(aq)	1.59617E-10	1.59617E-10	1.000	5.56405E-11	1.42903E-10	4.08760E-05	4.13E-09
H+	3.62542E-11	1.43493E-10	3.903	1.26396E-11	3.24579E-11	3.27143E-08	-4.92E-09
NpO2(OH)2-	1.42922E-12	4.26707E-13	0.2986	4.98278E-13	1.27956E-12	3.87785E-07	9.06E-09
HCl(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.49E+02
NaOH(aq)	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.94E+02
NpO2OH(aq)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.07E+00
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	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.25E-01
NaHCO3	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.26E+00
Na2CO3.10H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.70E+00
Na2CO3.7H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.74E+00
Na2CO3.H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
NaH(CO3)2.2H2O	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.28E+00

```

1775 pH (-log[ah+]); pmH(-log[mH+]) 9.8493 10.4406
1776 Osmotic Coefficient= 1.240893
1777 Equilibrium RH (%) = 77.824851
1778 Ionic Strength (m) = 5.615126
1779 Density, kg/m3 = 1188.79
1780 fCO2(g); log(fCO2(g)) = 4.873E-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= -4.64072887E+01
1791 Flashing Titration # 14
1792 # inversions for batch pblm 28
1793 Benchmark TITRATE Problem: Np(V)O2 with CO3 in 5.6molal NaCl FWT V2.3
1794 DATABASE: IHW84/FW86; Np(V)-Na-CO3-OH-Cl-C104 (NR94);
1795 95.01.31 Am(III)-Na-Cl-CO3-OH-PO4 (FRS89,FRF90,P91,RFFR92,RFF94,RUFF94)
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 3.89315740E+01 1.11018923E+02 9.93971848E+01 1.00182423E+05 Hydrogen
1802 3.68623841E+01 5.55624876E+01 4.97460678E+01 7.95907236E+05 Oxygen
1803 5.44291328E+00 5.61007250E+00 5.02279611E+00 1.15472927E+05 Sodium
1804 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1805 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
1806 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
1807 1.95518371E+00 5.57548454E+00 4.99182890E+00 1.76975310E+05 Chlorine
1808 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1809 3.46184645E+00 1.78114275E-02 1.59468828E-02 1.91538009E+02 Carbon
1810 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1811 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Nitrogen
1812 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Neon
1813 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Argon
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 Beryllium
1816 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Thallium
1817 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Lead
1818 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bismuth
1819 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Uranium
1820 3.47561578E+00 4.37689260E-05 3.91870854E-05 9.28922811E+00 Np(V)
1821 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 ClO4(-)
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 -1.51219098E-15 -4.31222774E-15 -3.86081298E-15 0.00000000E+00 Charge
1825
1826 Solution Parameters, Calculated
1827 SOLUTION MASS 465.601411995302 grams
1828 H2O MASS 350.675119778128 grams
1829 TDS(g/kg) 327.728674591707 g/kgH2O
1830
1831 Specified Solution Density
1832 DENSITY 1188.73872363963 kg/m3 = g/l
1833
1834 Solution Parameters Based on Specified Density
1835 SOLUTION VOL 0.391676827494728 liters
1836 TDS 293.421219101151 g/l
1837
1838 Density based on TDS and NaCl solutions 1188.73872363963 g/l
1839 Percent relative error vs NaCl density 0.000000000000000000 %
1840
1841
1842
1843

```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.32061E-01	7.78697E-01	0.9359	1.94655E+01	4.96997E+01	8.95318E+05	
NaH2PO4(aq)	9.91117E+00	1.00000E+00	1.000	3.47540E+00	8.87364E+00	3.12393E+06	
Na+	5.61007E+00	5.28007E+00	0.9413	1.96731E+00	5.02280E+00	1.15473E+05	
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"

```

1851 CO3+ CO3+ 1.64154E-02 4.25477E-04 2.5920E-02 5.75647E-03 1.46970E-03 8.81954E+02
1852 HCO3- HCO3- 1.27533E-03 4.76018E-04 0.3690 4.47227E-04 1.14183E-03 6.96708E+01
1853 OH- OH- 2.84255E-04 1.54941E-04 0.5451 9.96810E-05 2.54498E-04 4.32832E+00
1854 HPO2(CO3)3-- HPO2(CO3)3-- 3.32871E-05 2.77755E-14 8.3442E-10 1.16730E-05 2.98025E-05 1.33836E+01
1855 HPO2(CO3)2-- HPO2(CO3)2-- 1.03462E-05 2.72515E-10 2.6339E-05 3.62817E-06 9.26318E-06 3.60398E+00
1856 HPO2CO3- HPO2CO3- 1.34242E-07 2.43528E-07 1.814 4.70755E-08 1.20190E-07 3.95491E-02
1857 CO2(aq) CO2(aq) 2.29199E-08 6.65708E-08 2.904 0.03745E-09 2.05208E-08 6.03108E-04
1858 HPO2+ HPO2+ 1.17432E-09 2.10838E-09 1.966 4.11806E-10 1.05139E-09 2.82874E-04
1859 HPO2OH(aq) HPO2OH(aq) 1.38078E-10 1.28078E-10 1.000 4.84205E-11 1.23624E-10 3.53618E-05
1860 H+ H+ 1.31074E-11 5.06456E-11 3.864 4.59644E-12 1.17352E-11 1.18280E-06
1861 HPO2(OH)2- HPO2(OH)2- 2.46327E-12 1.03185E-12 0.2979 1.21448E-12 3.10072E-12 9.39710E-07
1862 HCl(aq) .....to titrate.acid.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1863 NaOH(aq) .....to titrate.base.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1864 HPO2OH(aq) HPO2OH(aq) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1865 HPO2OH(amor) HPO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1866 Na3HPO2(CO3)2(s)_DISABLED_DISABLED 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1867 NaCl Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1868 NaHCO3 NaHCO3 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1869 Na2CO3.10H2O Natron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1870 Na2CO3.7H2O Na2CO3-Heptahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1871 Na2CO3.H2O Throna 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1872 Na3H(CO3)2.2H2O Trona 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1873
1874 pH (-log(aH+)); pOH(-log(aOH)) 10.2955 10.8825
1875 Osmotic Coefficient= 1.239297
1876 Equilibrium RH (%) = 77.859707
1877 Ionic Strength (m) = 5.626852
1878 Density, kg/m3 = 1188.74
1879 fCO2(g); log{fCO2(g)} = 2.019E-06 -5.89
1880
1881 NOTES: - Water "molarity" is mole fraction H2O in aqueous phase
1882 - Gas "molarity" and "activity" are gas partial pressures
1883 - "Descriptor" means:
1884 *dg/RT*ln10 for species with nonzero concs. (convergence criterion)
1885 *Saturation Index for minerals, SI=log10(IAP/Ksp)
1886 *log10(activity) for aqueous species with very small concentrations
1887 *log10(partial pressure) for gases
1888
1889 Total G/RT= -4.65384402E+03
1890 Flashing Titration # 15
1891 # Inversions for batch pbm 28
1892 Benchmark TITRATE Problem: HPO2 with CO3 in 5.61molal NaCl Pmt V2.3
1893 DATABASE: HWR94/FWR95; HPO2-Na-CO3-OH-Cl-CO2 (HWR94);
1894 95.01.31 Am(III)-Na-Cl-CO3 (FWR95); IPR94; FPR94; RFF92; RFF94; RFF94;
1895 Pressure= 1.00000E+00 (=) ATM Temperature= 2.98E+02 (=) Kelvin
1896
1897 Elemental Abundances for Flash Problem
1898
1899 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter
1900
1901 3.95867206E+01 1.11018649E+02 9.94062598E+01 1.00191568E+05 Hydrogen
1902 3.72251652E+01 5.56624986E+01 4.98398335E+01 7.9740743E+05 Oxygen
1903 5.47601956E+00 5.61035435E+00 5.02347422E+00 1.15488517E+05 Sodium
1904 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1905 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Magnesium
1906 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Calcium
1907 1.9448480E+00 5.50989354E+00 4.9335227E+00 1.74908155E+05 Chlorine
1908 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Sulfur
1909 3.49364905E+00 5.08618173E-02 4.55413352E-02 5.46996977E+02 Carbon
1910 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Potassium
1911 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Negligion
1912 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Alr
1913 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron
1914 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Bromine
1915 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 TracerFl
1916 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Th(IV)
1917 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Am(III)
1918 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 U(VI)
1919 3.47151578E-04 2.88102498E-04 2.57965074E-04 6.12511564E+01 Hg(VI)
1920 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 ClO4- (EL)
1921 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Phosphorus
1922 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Electron
1923 -1.39330821E-15 -3.90748680E-15 -3.49873787E-15 0.00000000E+00 Charge
1924
1925 Solution Parameters, Calculated
1926 SOLUTION MASS 473.339684533624 grams
1927 H2O MASS 356.574003417585 grams
1928 TDS(g/kg) 127.465491025420 g/kgH2O
1929
1930 Specified Solution Density 1188.6038111845 kg/m^3 = g/l
1931 DENSITY
1932
1933 Solution Parameters Based on Specified Density
1934 SOLUTION VOL 0.398231666549673 liters
1935 TDS 293.210437350980 g/l
1936
1937 Density based on TDS and NaCl solutions 1188.6038111845 g/l
1938 Percent relative error vs NaCl density 0.000000000000000E+00 %
1939
1940
1941 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1942
1943 Species Name Molality Activity Act Coef Total Moles Molarity mg/liter Descriptor
1944
1945 H2O WATER 8.32465E-01 7.79962E-01 0.9369 1.97930E+01 4.97021E+01 8.95393E+05
1946 NaHPO2(CO3)3(s) NaHPO2(CO3)3(s) 9.74696E+00 1.00000E+00 1.000 3.47551E+00 8.72736E+00 3.07243E+06
1947 Na+ Na+ 5.61035E+00 5.26665E+00 0.9387 2.00051E+00 5.02347E+00 1.15489E+05
1948 Cl- Cl- 5.50989E+00 5.13884E+00 0.9327 1.94484E+00 4.93352E+00 1.74908E+05
1949 CO3= CO3= 4.81971E-02 1.24807E-03 2.5788E-02 1.72571E-02 4.31344E-02 2.60046E+03
1950 HCO3- HCO3- 1.63010E-03 5.97114E-04 0.3663 5.81251E-04 1.45958E-04 8.90593E+01
1951 OH- OH- 6.55397E-04 3.58792E-04 0.5474 2.33698E-04 5.86839E-04 9.98054E+00
1952 HPO2(CO3)3-- HPO2(CO3)3-- 2.58546E-04 2.39623E-13 9.2681E-10 9.21906E-05 2.31500E-04 1.03961E+02
1953 HPO2(CO3)2-- HPO2(CO3)2-- 2.94209E-05 8.01487E-10 2.7442E-05 1.04907E-05 2.63433E-05 1.02493E+01
1954 HPO2CO3- HPO2CO3- 1.35468E-07 2.46132E-07 1.802 4.83043E-08 1.21297E-07 3.99135E-02
1955 CO2(aq) CO2(aq) 1.35492E-08 3.64751E-08 2.907 4.4742E-09 1.12365E-08 4.94515E-04
1956 HPO2+ HPO2+ 4.11022E-10 7.89015E-10 1.920 1.46560E-10 3.68027E-10 9.90165E-05
1957 HPO2OH(aq) HPO2OH(aq) 1.09291E-10 1.09291E-10 1.000 3.89705E-11 9.78589E-11 2.79929E-05
1958 HPO2(OH)2- HPO2(OH)2- 6.38945E-12 1.89128E-12 0.2960 2.27811E-12 5.72107E-12 1.73384E-06
1959 H+ H+ 5.83772E-12 2.19066E-11 3.756 2.07880E-12 5.23256E-12 5.26384E-09
1960 HCl(aq) .....to titrate.acid.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1961 NaOH(aq) .....to titrate.base.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1962 HPO2OH(aq) HPO2OH(aq) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1963 HPO2OH(amor) HPO2OH(amor) 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1964 Na3HPO2(CO3)2(s)_DISABLED_DISABLED 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1965 NaCl Halite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1966 NaHCO3 NaHCO3 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1967 Na2CO3.10H2O Natron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1968 Na2CO3.7H2O Na2CO3-Heptahydrate 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1969 Na2CO3.H2O Throna 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1970 Na3H(CO3)2.2H2O Trona 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00
1971
1972 pH (-log(aH+)); pOH(-log(aOH)) 10.6594 11.2341
1973 Osmotic Coefficient= 1.234823
1974

```

Appendix O: Sample Output File "Np_NaCl_BM.OUT"

```
1975 Equilibrium RH (%) = 77.996177
1976 Ionic Strength (m) = 5.461425
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 *Q/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:(SCBASS.FWT.UN)NP_NACL_BM.TITRATE;2
```

Appendix P: Sample Output File "BATCH_DOC.FOR088"

See Table 16 for explanation of this listing

Line	Sample Output	Reference
1	5.55068155779565E+01 H2O	WATER 5.506118174079332E+01
2	0.016254633034410E-01 Na+	Na+ 2.00000000000000E-02
3	1.00812713512026E-02 K+	K+ 1.00000000000000E-02
4	1.00115409035505E-04 Ca++	Ca++ 9.92082987467669E-05
5	1.098734763517149E-08 Mg++	Mg++ 1.08976985023399E-08
6	3.542680237963029E-08 MgOH+	MgOH+ 3.51411986301455E-08
7	1.93211561795198E-13 H+	H+ 1.91653288621170E-13
8	1.108940051468925E-01 Cl-	Cl- 1.08999999999999E-01
9	1.00812713512026E-02 SO4-	SO4- 9.9999999999995E-04
10	4.06798652328464E-15 HCO3-	HCO3- 9.80006626742278E-02
11	9.87965441186853E-02 OH-	OH- 1.09204419190607E-07
12	1.100939975666261E-07 HCO3-	HCO3- 9.9199126039683E-05
13	1.000053490322309E-04 CO3-	CO3- 2.19359632439379E-14
14	2.211424382613913E-14 CO2(aq)	CO2(aq) 6.126147055515301E-07
15	6.972356792462450E-07 CaCO3(aq)	CaCO3(aq) 5.279149790344147E-11
16	5.322055127469460E-11 MgCO3(aq)	MgCO3(aq) 1.64077085239343E-11
17	1.654105921210009E-11 B(OH)3(aq)	B(OH)3(aq) 9.98970524756217E-08
18	1.0077089477393209E-07 B(OH)4-	B(OH)4- 0.00000000000000E+00
19	0.00000000000000E+00 B(OH)4-	B(OH)4- 0.00000000000000E+00
20	0.00000000000000E+00 B(OH)4-	B(OH)4- 0.00000000000000E+00
21	6.723697139064127E-11 CaB(OH)4-	CaB(OH)4- 6.653368448780785E-11
22	6.18465924044248E-15 MgB(OH)4-	MgB(OH)4- 6.134836150463729E-15
23	0.00000000000000E+00 Br-	Br- 0.00000000000000E+00
24	0.00000000000000E+00 ClO4-	perchlorate ClO4- 0.00000000000000E+00
25	0.00000000000000E+00 NaOH(aq)	to titrate, base, only 0.00000000000000E+00
26	0.00000000000000E+00 HCl(aq)	to titrate, acid, only 0.00000000000000E+00
27	0.00000000000000E+00 HClO4(aq)	to titrate, acid, only 0.00000000000000E+00
28	0.00000000000000E+00 Pos(aq)	POSITIVE ION 0.00000000000000E+00
29	0.00000000000000E+00 NegIon	NEGATIVE ION 0.00000000000000E+00
30	0.00000000000000E+00 PosIon(OH)	to titrate, base 0.00000000000000E+00
31	0.00000000000000E+00 NegIon(aq)	to titrate, acid 0.00000000000000E+00
32	0.00000000000000E+00 Tracer(aq)	conservative tracer 0.00000000000000E+00
33	0.00000000000000E+00 H2PO4(aq)	H2PO4(aq) 0.00000000000000E+00
34	0.00000000000000E+00 H2PO4-	H2PO4- 0.00000000000000E+00
35	0.00000000000000E+00 HPO4--	HPO4-- 0.00000000000000E+00
36	0.00000000000000E+00 PO4---	PO4--- 0.00000000000000E+00
37	0.00000000000000E+00 HPO2+	HPO2+ 0.00000000000000E+00
38	0.00000000000000E+00 HPO2OH(aq)	HPO2OH(aq) 0.00000000000000E+00
39	0.00000000000000E+00 HPO2(OH)2-	HPO2(OH)2- 0.00000000000000E+00
40	0.00000000000000E+00 HPO2CO3-	HPO2CO3- 0.00000000000000E+00
41	0.00000000000000E+00 HPO2(CO3)2--	HPO2(CO3)2-- 0.00000000000000E+00
42	0.00000000000000E+00 HPO2(CO3)3---	HPO2(CO3)3--- 0.00000000000000E+00
43	0.00000000000000E+00 Am+++	Am+++ 0.00000000000000E+00
44	0.00000000000000E+00 AmCO3+	AmCO3+ 0.00000000000000E+00
45	0.00000000000000E+00 Am(CO3)2-	Am(CO3)2- 0.00000000000000E+00
46	0.00000000000000E+00 Am(CO3)3--	Am(CO3)3-- 0.00000000000000E+00
47	0.00000000000000E+00 Am(OH)2+	Am(OH)2+ 0.00000000000000E+00
48	0.00000000000000E+00 Am(OH)3(aq)	Am(OH)3(aq) 0.00000000000000E+00
49	0.00000000000000E+00 Th+++	Th+++ 0.00000000000000E+00
50	0.00000000000000E+00 UO2++	U(VI)O2++ 0.00000000000000E+00
51	0.00000000000000E+00 NpO2OH(aged)	NpO2OH(aged) 0.00000000000000E+00
52	0.00000000000000E+00 NpO2OH(amor)	NpO2OH(amor) 0.00000000000000E+00
53	0.00000000000000E+00 NpO2CO3(s)	NpO2CO3(s) 0.00000000000000E+00
54	0.00000000000000E+00 Na3NpO2(CO3)3(a) DTABLED DTABLED	Na3NpO2(CO3)3(a) 0.00000000000000E+00
55	0.00000000000000E+00 AmOHCO3(c)	AmOHCO3(c) 0.00000000000000E+00
56	0.00000000000000E+00 Am(OH)3(s)	Am(OH)3(s) 0.00000000000000E+00
57	0.00000000000000E+00 NaAm(CO3)2.6H2O(c)	NaAm(CO3)2.6H2O(c) 0.00000000000000E+00
58	0.00000000000000E+00 AmPO4(c)	AmPO4(c) 0.00000000000000E+00
59	0.00000000000000E+00 CsSO4	Amphibrite 0.00000000000000E+00
60	0.00000000000000E+00 NaK3(SO4)2	Aphthitalite/Glaucarite 0.00000000000000E+00
61	0.00000000000000E+00 CaCl2.6H2O	Antarcticite 0.00000000000000E+00
62	0.00000000000000E+00 CaCO3	Aragonite 0.00000000000000E+00
63	0.00000000000000E+00 K2SO4	Arkanite 0.00000000000000E+00
64	0.00000000000000E+00 MgCl2.6H2O	Bischofite 0.00000000000000E+00
65	0.00000000000000E+00 Mg(SO4)2.4H2O	Brewite 9.99539072134877E-04
66	1.00888952140455E-03 Mg(OH)2	Burkellite 0.00000000000000E+00
67	0.00000000000000E+00 Na6CO3(SO4)2	Calcite 0.00000000000000E+00
68	0.00000000000000E+00 CaCO3	CaCl2.Tetrahedrite 0.00000000000000E+00
69	0.00000000000000E+00 CaCl2.4H2O	CaOxychloride A 0.00000000000000E+00
70	0.00000000000000E+00 Ca4Cl2(OH)6.13H2O	CaOxychloride B 0.00000000000000E+00
71	0.00000000000000E+00 Ca2Cl2(OH)2.H2O	Carrollite 0.00000000000000E+00
72	0.00000000000000E+00 KMgCl3.6H2O	Epsomite 0.00000000000000E+00
73	0.00000000000000E+00 MgSO4.7H2O	Gaylussite 0.00000000000000E+00
74	0.00000000000000E+00 CaNa2(CO3)2.5H2O	Glauberite 0.00000000000000E+00
75	0.00000000000000E+00 Na2Ca(SO4)2	Gypsum 0.00000000000000E+00
76	0.00000000000000E+00 CaSO4.2H2O	Halite 0.00000000000000E+00
77	0.00000000000000E+00 NaCl	Hexahydrite 0.00000000000000E+00
78	0.00000000000000E+00 MgSO4.6H2O	Kainite 0.00000000000000E+00
79	0.00000000000000E+00 KMgCl3O4.3H2O	Kalicinite 0.00000000000000E+00
80	0.00000000000000E+00 KNCO3	Kieserite 0.00000000000000E+00
81	0.00000000000000E+00 MgSO4.H2O	Leonite 0.00000000000000E+00
82	0.00000000000000E+00 K2Mg(SO4)2.4H2O	Lialite_Salt 0.00000000000000E+00
83	0.00000000000000E+00 Na4Ca(SO4)3.2H2O	Magnesite 0.00000000000000E+00
84	0.00000000000000E+00 MgCO3	MgOxychloride 0.00000000000000E+00
85	0.00000000000000E+00 Mg2Cl(OH)3.4H2O	Mercallite 0.00000000000000E+00
86	0.00000000000000E+00 KHSO4	Mirabilite 0.00000000000000E+00
87	0.00000000000000E+00 Na2SO4.10H2O	Muscovite 0.00000000000000E+00
88	0.00000000000000E+00 KHS(SO4)7	Nalite 0.00000000000000E+00
89	0.00000000000000E+00 NaHCO3	Nahcolite 0.00000000000000E+00
90	0.00000000000000E+00 Na2CO3.10H2O	Metron 0.00000000000000E+00
91	0.00000000000000E+00 MgCO3.3H2O	Nesquehonite 0.00000000000000E+00
92	0.00000000000000E+00 K2Mg(SO4)2.6H2O	Picromerite/Schoen 0.00000000000000E+00
93	0.00000000000000E+00 Na2Ca(CO3)2.2H2O	Piresonite 0.00000000000000E+00
94	0.00000000000000E+00 K2MgC2(OH)4.2H2O	Polynilite 0.00000000000000E+00
95	0.00000000000000E+00 Ca(OH)2	Portlandite 0.00000000000000E+00
96	0.00000000000000E+00 K2CO3.3/2H2O	Potassium Carbonate 0.00000000000000E+00
97	0.00000000000000E+00 KHS4(CO3)6.3H2O	K-Segulcarbonate 0.00000000000000E+00
98	0.00000000000000E+00 KH2CO3.6H2O	K-Na-Carbonate 0.00000000000000E+00
99	0.00000000000000E+00 K2NaH(CO3)2.2H2O	Potassium Trona 0.00000000000000E+00
100	0.00000000000000E+00 K3H(SO4)2	Sesquipotassium Sulfate 0.00000000000000E+00
101	0.00000000000000E+00 Na3H(SO4)2	Sesquisodium Sulfate 0.00000000000000E+00
102	0.00000000000000E+00 Na2CO3.7H2O	Na2CO3-Heptahydrate 0.00000000000000E+00
103	0.00000000000000E+00 KCl	Sylvite 0.00000000000000E+00
104	0.00000000000000E+00 K2Ca(SO4)2.H2O	Syngonite 0.00000000000000E+00
105	0.00000000000000E+00 Mg2CaCl6.12H2O	Tachyhydrite 0.00000000000000E+00
106	0.00000000000000E+00 Na2SO4	Thénardite 0.00000000000000E+00
107	0.00000000000000E+00 Na2CO3.H2O	Thermonatrite 0.00000000000000E+00
108	0.00000000000000E+00 Na3H(CO3)2.2H2O	Trona 0.00000000000000E+00
109	0.00000000000000E+00 Na2B4O7.10H2O	Borax 0.00000000000000E+00
110	0.00000000000000E+00 B(OH)3	Borix Acid Solid 0.00000000000000E+00
111	0.00000000000000E+00 KB5O8.4H2O	K-Pentaborate_(10_C) 0.00000000000000E+00
112	0.00000000000000E+00 KB4O7.4H2O	K-Tetraborate_(10_C) 0.00000000000000E+00
113	0.00000000000000E+00 Na2B2O4.4H2O	Sodium Metaborate 0.00000000000000E+00
114	0.00000000000000E+00 Na2B5O8.5H2O	Sodium Pentaborate 0.00000000000000E+00

Appendix P: Sample Output File

INFORMATION ONLY

115 0.0000000000000000E+00 NaBO2.NaCl.2H2O_Template_(20_C) 0.0000000000000000E+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	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	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	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	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	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	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	0.00000E+00
246									
247	0)	IonicStrength	Titrvol.ml			pH			pOH
248	1)	5.61119E+00	0.000000000E+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			9.915
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(VI)O2 with CO3 in 5.61molar NaCl FMT V2.3
2 DATABASE: H0404/0404; Np(VI)-Na-Cl-CO3-04-04 (H0404) (H0404)
3 05.01.11 Am(111)-Na-Cl-CO3-04-04 (FR889,FR90,91,92,93,94,95,96)

Titrant Volumes per Grid Block, in milliliters										
1	0.000000	ml.								
2	0.100000	ml.								
3	0.200000	ml.								
4	0.300000	ml.								
5	0.400000	ml.								
6	0.500000	ml.								
7	0.600000	ml.								
8	0.700000	ml.								
9	0.800000	ml.								
10	0.900000	ml.								
11	1.000000	ml.								
12	1.100000	ml.								
13	1.200000	ml.								
14	1.300000	ml.								
15	1.400000	ml.								

Titration Results, molar										
01	HCO3	Na+	Z+	Ca++	Mg++	MgOH+	H+	Cl-	SO4+	
11	1.92928E+01	5.61057E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.21872E-05	5.61096E+00	0.00000E+00	
21	1.92778E+01	5.61014E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.77300E-05	5.60992E+00	0.00000E+00	
31	1.93027E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.87409E-09	5.60892E+00	0.00000E+00	
41	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	
51	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	
61	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	
71	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	
81	1.93277E+01	5.61001E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	6.42959E-11	5.60375E+00	0.00000E+00	
91	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	
101	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	
111	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	
121	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	
131	1.93527E+01	5.61002E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.60509E-11	5.59858E+00	0.00000E+00	
141	1.93577E+01	5.61002E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.30838E-11	5.59754E+00	0.00000E+00	
151	1.93627E+01	5.61002E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.06048E-11	5.59650E+00	0.00000E+00	

Titration Results, molar (continued)										
01	HCO3-	OH-	HCO3-	CO3-	CO2(aq)	CaCO3(aq)	MgCO3(aq)	H(OH)3(aq)	H(OH)4-	
11	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	
21	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	
31	0.00000E+00	9.49192E-09	4.25147E-04	5.36072E-06	4.16260E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
41	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	
51	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	
61	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	
71	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	
81	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	
91	0.00000E+00	6.42010E-05	1.06274E-03	3.07597E-03	8.53187E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
101	0.00000E+00	7.38545E-05	1.07118E-03	3.58175E-03	7.44762E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
111	0.00000E+00	8.35411E-05	1.08042E-03	4.08730E-03	6.64082E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
121	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	
131	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	
141	0.00000E+00	1.11678E-04	1.10821E-03	5.60253E-03	5.09071E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
151	0.00000E+00	1.20769E-04	1.11706E-03	6.10711E-03	4.74407E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	

Titration Results, molar (continued)										
01	Br-	ClO4-	NaOH(aq)	HCl(aq)	HClO4(aq)	HCO3-	HCO3-	HCO3-	HCO3-	
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	
21	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
31	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
41	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
51	0.00000E+00	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	0.00000E+00	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	0.00000E+00	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	0.00000E+00	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	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
101	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
111	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
121	0.00000E+00	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	0.00000E+00	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	0.00000E+00	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	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	

Titration Results, molar (continued)										
01	PosIon	MgIon	PosIon(OH)	MgIon(OH)	Tracer	H3PO4(aq)	H2PO4-	HPO4-	PO4--	
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	
21	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
31	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
41	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
51	0.00000E+00	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	0.00000E+00	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	0.00000E+00	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	0.00000E+00	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	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
101	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
111	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
121	0.00000E+00	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	0.00000E+00	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	0.00000E+00	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	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	

Titration Results, molar (continued)										
01	NpO2+	NpO2OH(aq)	NpO2(OH)2-	NpO2CO3-	NpO2(CO3)2--	NpO2(CO3)3---	Am+++	AmCO3+	Am(CO3)2-	
11	6.12705E-04	4.57851E-10	2.04218E-16	1.33526E-07	1.98384E-11	1.25197E-16	0.00000E+00	0.00000E+00	0.00000E+00	
21	6.12705E-04	4.57851E-10	2.04218E-16	1.33526E-07	1.98384E-11	1.25197E-16	0.00000E+00	0.00000E+00	0.00000E+00	
31	4.62427E-07	1.76885E-10	1.47303E-14	1.33612E-07	2.72677E-08	2.35800E-10	0.00000E+00	0.00000E+00	0.00000E+00	
41	4.67707E-08	1.73300E-10	1.81034E-13	1.33612E-07	3.48878E-07	3.85776E-08	0.00000E+00	0.00000E+00	0.00000E+00	
51	4.67707E-08	1.73300E-10	1.81034E-13	1.33612E-07	3.48878E-07	3.85776E-08	0.00000E+00	0.00000E+00	0.00000E+00	
61	1.22005E-08	1.69754E-10	4.97012E-13	1.33612E-07	9.97249E-07	3.14830E-07	0.00000E+00	0.00000E+00	0.00000E+00	
71	9.23118E-09	1.68120E-10	6.45975E-13	1.33612E-07	1.32681E-06	5.51917E-07	0.00000E+00	0.00000E+00	0.00000E+00	
81	7.40667E-09	1.65532E-10	7.89467E-13	1.33710E-07	1.64391E-06	8.54484E-07	0.00000E+00	0.00000E+00	0.00000E+00	
91	6.18630E-09	1.65046E-10	9.27455E-13							

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		pH	
248	1)	5.61119E+00	0.00000000E+00		5.320		5.914	
249	2)	5.61031E+00	0.10000000		5.645		6.239	
250	3)	5.61004E+00	0.20000000		7.818		8.412	
251	4)	5.61055E+00	0.30000000		8.917		9.510	
252	5)	5.61106E+00	0.40000000		9.198		9.791	
253	6)	5.61157E+00	0.50000000		9.364		9.957	
254	7)	5.61208E+00	0.60000000		9.482		10.07	
255	8)	5.61259E+00	0.70000000		9.573		10.17	
256	9)	5.61310E+00	0.80000000		9.647		10.24	
257	10)	5.61362E+00	0.90000000		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)	5.61515E+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"

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		pmt	
248	1)	5.61119E+00	0.000000000E+00		5.320		5.914	
249	2)	5.61031E+00	0.100000000		5.645		6.239	
250	3)	5.61008E+00	0.142510000		5.994		6.587	
251	4)	5.61003E+00	0.160000000		6.235		6.829	
252	5)	5.61001E+00	0.180000000		6.700		7.293	
253	6)	5.61006E+00	0.203090000		7.943		8.536	
254	7)	5.61014E+00	0.220000000		8.332		8.925	
255	8)	5.61024E+00	0.240000000		8.565		9.159	
256	9)	5.61034E+00	0.260000000		8.717		9.310	
257	10)	5.61049E+00	0.289430000		8.872		9.465	
258	11)	5.61119E+00	0.412460000		9.222		9.815	
259	12)	5.61202E+00	0.587800000		9.469		10.06	
260	13)	5.61513E+00	1.19380000		9.849		10.44	
261	14)	5.62685E+00	3.45510000		10.30		10.88	
262	15)	5.66143E+00	10.0000000		10.66		11.23	

Appendix T: Command File FMT_CUR.COM

```
1 $! SET noverify
2 $! SET verify
3 $! FMT_CUR.COM assigns and fetches user-selected
4 $! chemdat and rhomin data base file names,
5 $! assign user-specified input/output file names,
6 $! executes fmt-fmt in CMS 1997 nonPA (Performance
7 $! Assessment) production area
8 $! Copied from FMT_FMTC.COM
9 $!
10 $! Modifier: S. C. Babb
11 $! Date: 03/31/97
12 $! Reason: query user on PRINT/NOPRINT chemdat db in OUT file
13 $! set executable to fmt vs2.3
14 $!
15 $! Modifier: S. C. Babb
16 $! Date: 04/29/97
17 $! Reason: write input/output filenames and linker information
18 $! to log file
19 $!
20 $! *****
21 $!
22 $! INPUTS:
23 $!
24 $! P1 - Substring chemdat file name search on valance states, dates,
25 $! and/or fugacity
26 $!
27 $! P2 - Substring rhomin file name search on valance states and/or dates
28 $!
29 $! P3 - Input File Name (no extension)
30 $!
31 $! P4 - Directory where Input Files located (optional)
32 $!
33 $! -----
34 $!
35 $!
36 $! Turn on error handling; exit on any error.
37 $!
38 $ ON error then goto error_exit
39 $ mode = f$mode()
40 $!
41 $! Logic flow
42 $!
43 $! Optional - Set P4 - this is the directory where input files are located,
44 $! SCMS files are fetched to and output files are generated
45 $!
46 $ IF p4 .nes. ""
47 $ THEN
48 $ set default 'p4'
49 $ ENDIF
50 $!
51 $ GOSUB check_filename
52 $ GOSUB define_cms_library
53 $ GOSUB delete_files
54 $ GOSUB get_database_files
55 $ GOSUB define_inputs
56 $ GOSUB define_outputs
57 $ GOSUB start_log
58 $! GOSUB start_mail
59 $ GOSUB run_fmt
60 $ GOSUB undefine_symbols
61 $ EXIT
```

Appendix T: Command File FMT_CUR.COM

```
62 $!-----  
63 $CHECK_FILENAME:  
64 $! Determine if any or all file names are passed as parameters. If not,  
65 $! prompt for one if this is an interactive session;  
66 $! otherwise flag an error and exit  
67 $!  
68 $! Check for P1 - this is the CHEMDAT name field  
69 $!  
70 $ IF mode .eqs. "BATCH" .and. p1 .eqs. ""  
71 $ THEN  
72 $ WRITE sys$output -  
73 $ "Can not run in batch without a chemdat file name (P1). exiting."  
74 $ GOTO error_exit  
75 $ ENDIF  
76 $!  
77 $!  
78 $ IF p1 .eqs. ""  
79 $ THEN  
80 $ INQUIRE chemdat_name -  
81 $ "Enter chemdat file name to search on"  
82 $ IF chemdat_name .eqs. "" THEN goto error_exit  
83 $ ELSE  
84 $ chemdat_name = p1  
85 $ ENDIF  
86 $!  
87 $! Check for P2 - this is the RHOMIN name field  
88 $!  
89 $ IF mode .eqs. "BATCH" .and. p2 .eqs. ""  
90 $ THEN  
91 $ WRITE sys$output -  
92 $ "Can not run in batch without a rhomin file name (P2). exiting."  
93 $ GOTO error_exit  
94 $ ENDIF  
95 $!  
96 $!  
97 $ IF p2 .eqs. ""  
98 $ THEN  
99 $ INQUIRE rhomin_name -  
100 $ "Enter rhomin file name to search on"  
101 $ IF rhomin_name .eqs. "" THEN goto error_exit  
102 $ ELSE  
103 $ rhomin_name = p2  
104 $ ENDIF  
105 $!  
106 $! Check for P3 - this is the file name field  
107 $!  
108 $ IF mode .eqs. "BATCH" .and. p3 .eqs. ""  
109 $ THEN  
110 $ WRITE sys$output -  
111 $ "Can not run in batch without a file name (P3). exiting."  
112 $ GOTO error_exit  
113 $ ENDIF  
114 $!  
115 $!  
116 $ IF p3 .eqs. ""  
117 $ THEN  
118 $ INQUIRE file_name "Enter input file name (without .extension)"  
119 $ IF file_name .eqs. "" THEN goto error_exit  
120 $ ELSE  
121 $ file_name = p3  
122 $ ENDIF  
123 $ RETURN  
124 $!-----
```


Appendix T: Command File FMT_CUR.COM

```
125 $DEFINE_CMS_LIBRARY:
126 $! Define non-pa cms symbols and point to fmt library
127 $!
128 $! set noverify
129 $ nonpa_cms_syms
130 $!
131 $! Set CMS library to FMT
132 $!
133 $ cms_library_name = "fmt"
134 $ lib'cms_library_name
135 $! set verify
136 $!
137 $ RETURN
138 $! -----
139 $DEFINE_INPUTS:
140 $! Define the input files needed.
141 $!
142 $ DEFINE input 'file_name'.in
143 $ DEFINE inguess 'file_name'.inguess
144 $!
145 $! Define a logical that points to the database files just fetched
146 $!
147 $ DEFINE chemdat 'chemdat_name'
148 $ DEFINE rhomin 'rhomin_name'
149 $!
150 $ RETURN
151 $! -----
152 -
153 $DEFINE_OUTPUTS:
154 $! Define the output files needed.
155 $!
156 $ DEFINE output 'file_name'.out
157 $ DEFINE for088 'file_name'.for088
158 $ DEFINE titrate 'file_name'.titrate
159 $!
160 $ RETURN
161 $! -----
162 -
163 $DELETE_FILES:
164 $!
165 $! Turn off warning messages for no files to delete
166 $!
167 $ SET noon
168 $ SET message/nofac/nosev/notext/noid
169 $! Delete all 'file_name'.moles files; do not accumulate them.
170 $!
171 $ DELETE 'file_name'.moles;*
172 $! Delete all fmt prefixed files of chemdat and rhomin files
173 $!
174 $ DELETE fmt_*.chemdat;*
175 $ DELETE fmt_*.rhomin;*
176 $ SET message/fac/sev/text/id
177 $ SET on
178 $!
179 $ RETURN
180 $! -----
181 -
182 $ERROR_EXIT:
183 $! Exit routine when a severe error is encountered.
184 $!
185 $ Write sys$output "Executing error exit, '$status'."
186 $ EXIT
```

INFORMATION ONLY

Appendix T: Command File FMT_CUR.COM

```
187 $! -----
188 -
189 $GET_DATABASE_FILES:
190 $!
191 $! If interactive, allow user to select/pick from a list of chemdat file names
192 $!
193 $ IF mode .nes. "BATCH"
194 $ THEN
195 $   cse "'chemdat_name'*.chemdat"
196 $!
197 $   INQUIRE chemdat_name "Select CHEMDAT name from list above"
198 $ ENDIF
199 $!
200 $! Fetch chemdat from FMT CMS
201 $!
202 $!   set noverify
203 $   cfe 'chemdat_name'
204 $!   set verify
205 $!
206 $! If interactive allow user to select/pick from a list of rhomin file names
207 $!
208 $ IF mode .nes. "BATCH"
209 $ THEN
210 $   cse "'rhomin_name'*.rhomin"
211 $!
212 $   INQUIRE rhomin_name "Select RHOMIN name from list above"
213 $ ENDIF
214 $!
215 $! Fetch chemdat from FMT CMS
216 $!   set noverify
217 $   cfe 'rhomin_name'
218 $!   set verify
219 $!
220 $ RETURN
221 $! -----
222 -
223 $RUN_FMT:
224 $!
225 $! Write the image information in the log file
226 $! Define the run symbols needed.
227 $   define /nolog exe_dir
228 wp$nonpa_prodroot:[fmt.exe]
229 $   fmt ::= "$exe_dir:fmt_pa97.exe"
230 $!
231 $! Run the utility that shows image information from the exe. (mandatory!)
232 $! This is part of the documentation required while doing a calculation.
233 $ @wp$ref:wp_get_image_id.com
234 exe_dir:fmt_pa97.exe
235 $!
236 $! Get user input for print/noprint of chemdat parameters in the out file
237 $! define/user sys$input sys$command
238 $   inquire answer "Enter "Y" or "y" to echo database in OUT file"
239 $!
240 $   if answer .eqs. "Y" then goto close_log_file
241 $   if answer .eqs. "y" then goto close_log_file
242 $   write sys$output "Pitzer Data Base NOT echoed in this Run"
243 $close_log_file:
244 $   deassign sys$output
245 $!
246 $! Write information to the user's screen
247 $! Run the utility that shows image information from the exe. (mandatory!)
248 $! This is part of the documentation required while doing a calculation.
```

Appendix T: Command File FMT_CUR.COM

```
249 $ @wp$ref:wp_get_image_id.com
250 exe_dir:fmt_pa97.exe
251 $!
252 $! Run the code
253 $ . fmt 'answer'
254 $ RETURN
255 $! -----
256 -
257 $START_LOG:
258 $!
259 $!
260 $ month == f$cvtime("'f$time()'", "absolute", "month" )
261 $ day == f$cvtime("'f$time()'", "comparison", "day" )
262 $ hour == f$cvtime("'f$time()'", "absolute", "hour" )
263 $ min == f$cvtime("'f$time()'", "absolute", "minute" )
264 $!
265 $ log_file_name := "'file_name'_'month'_'day'_'hour'_'min'.log"
266 $! mike williamson's log file definition:
267 $! "sys$login:fmt_'file_name'_'month'_'day'_'hour'_'min'.log"
268 $!
269 $ DEFINE/proc sys$output 'log_file_name
270 $! Write the input file names
271 $ show logical input
272 $ show logical inguess
273 $! Write the data base file names
274 $ show logical chemdat
275 $ show logical rhomin
276 $! Write the output file names
277 $ show logical output
278 $ show logical for088
279 $ show logical titrate
280 $!
281 $ RETURN
282 $! -----
283 $START_MAIL:
284 $! Open a file where we can write a message that can be sent to the
285 $! user upon completion.
286 $!
287 $ mail_error_flag = 0
288 $ mail_file_name := "sys$login:fmt_mail.msg"
289 $ mail_subject := "FMT 'file_name' run."
290 $ mail_list == f$getjpi( "", "username")
291 $!
292 $ OPEN/write mail_file 'mail_file_name
293 $!
294 $ RETURN
295
296 $! -----
297 -
298 $TERMINATE:
299 $! If there was no previously flagged error or problem, search the log files
300 $! for any fatal, error, or warning messages.
301 $!
302 $! Deassign sys$output so the "log" file closes.
303 $ deassign sys$output
304 $!
305 $! Show the run output to the user
306 $ TYPE 'log_file_name
307 $!
308 $! Skip sending the mail message
309 $ goto end_terminate
310 $!
311 $! If there was not a previous error recorded, search the log file for
```

Appendix T: Command File FMT_CUR.COM

```
312 $! common error indicators.
313 $ search_status = 0
314 $ IF mail_error_flag .ne. 1
315 $ THEN
316 $! Turn off informational messages from search command
317 $ SET message/nofac/nosev/notext/noid
318 $ SEARCH 'log_file_name "-F-","-E-","-W-" / match=or
319 $ search_status = $status
320 $! Turn on messages
321 $ SET message/fac/sev/text/id
322 $ ENDIF
323 $!
324 $ IF search_status .eq. 1 .or. mail_error_flag .eq. 1
325 $ THEN
326 $ WRITE mail_file "The run log contains an error or warning. "
327 $ WRITE mail_file "Please examine 'log_file_name'."
328 $ mail_subject == "'mail_subject' ERROR"
329 $ ELSE
330 $ WRITE mail_file "The FMT run has completed."
331 $ ENDIF
332 $!
333 $ CLOSE/nolog mail_file
334 $ MAIL/subject="'mail_subject'" 'mail_file_name 'mail_list
335 $!
336 $END_TERMINATE:
337 $ EXIT
338 $!-----
339 $UNDEFINE_SYMBOLS:
340 $! Deassign input files
341 $!
342 $ DEASSIGN input
343 $ DEASSIGN inguess
344 $ DEASSIGN chemdat
345 $ DEASSIGN rhomin
346 $ DEASSIGN output
347 $ DEASSIGN for088
348 $ DEASSIGN titrate
349 $!
350 $ RETURN
351 $!-----
352 -
353 $! CMS REPLACEMENT HISTORY, Element FMT_FMTC.COM
354 $! *3 23-SEP-1996 09:09:31 SCBABB "ADD PARAMETER P4 FOR BATCH RUNS"
355 $! *2 21-DEC-1995 12:58:57 SCBABB "FMT EXECUTABLE NAME CHANGED"
356 $! *1 19-DEC-1995 12:26:54 SCBABB "USER COMMAND FILE FOR EXECUTING
357 FMT_FMT2P0 FROM CMS"
358 $! CMS REPLACEMENT HISTORY, Element FMT_FMTC.COM
```


Appendix U: Derivation of CO₂ Fugacity

The derivation of the expression for calculating for CO₂ (g) fugacity within FMT is given below.

The CO₂ equilibrium reaction can be written as:



The equilibrium expression corresponding to this reaction is

$$K^{\text{eq}} = \frac{(a_{\text{H}^+})^2 (a_{\text{CO}_3^{2-}})}{f_{\text{CO}_2(\text{g})} a_{\text{H}_2\text{O}}} \quad (2)$$

Taking the log₁₀ of this expression and rearranging terms yield

$$\log f_{\text{CO}_2(\text{g})} = 2 \log a_{\text{H}^+} + \log a_{\text{CO}_3^{2-}} - \log a_{\text{H}_2\text{O}} - \log K^{\text{eq}} \quad (3)$$

or, since $\text{pH} \equiv -\log a_{\text{H}^+}$,

$$\log f_{\text{CO}_2(\text{g})} = -2\text{pH} + \log a_{\text{CO}_3^{2-}} - \log a_{\text{H}_2\text{O}} - \log K^{\text{eq}} \quad (4)$$

The equilibrium constant, K^{eq} , is related to the free energy change of reaction, $\Delta G_{\text{RXN}}^\circ$, by the expression

$$K^{\text{eq}} = \exp\left(\frac{-\Delta G_{\text{RXN}}^\circ}{RT}\right) \quad (5)$$

The $\Delta G_{\text{RXN}}^\circ$ is related to the standard chemical potentials of the species shown in reaction equation 1 by the expression

$$\frac{\Delta G_{\text{RXN}}^\circ}{RT} = \frac{\mu_{\text{H}^+}^\circ}{RT} + \frac{\mu_{\text{CO}_3^{2-}}^\circ}{RT} - \frac{\mu_{\text{CO}_2(\text{g})}^\circ}{RT} - \frac{\mu_{\text{H}_2\text{O}}^\circ}{RT} \quad (6)$$

Substituting values for the standard chemical potentials, Equation 6 becomes

$$\frac{\Delta G_{\text{RXN}}^\circ}{RT} = 2(0) + (-212.944) - (-159.092) - (-95.6635) = 41.8115 \quad (7)$$

Therefore, $K^{\text{eq}} = 6.9422 \times 10^{-19}$, and $\log K^{\text{eq}} = -18.1585$.


The equation for the log₁₀ of CO₂ fugacity can be simplified to

$$\log f_{\text{CO}_2(\text{g})} = -2\text{pH} + \log a_{\text{CO}_3^{2-}} - \log a_{\text{H}_2\text{O}} + 18.1585 \quad (8)$$

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 contain 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⁺, Mg²⁺, OH⁻, Cl⁻, CO₃²⁻, and SO₄²⁻, 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.

Appendix V: Memorandum on Current Release of 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-SO₄-OH-HCO₃-CO₃-CO₂-H₂O; 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.

Appendix V: Memorandum on Current Release of Data Base

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

$$\frac{\overset{\circ}{\mu}}{RT}(\text{Pu(III) Species}) = -\frac{\overset{\circ}{\mu}}{RT}(\text{Am(III) Species}) + v \left(\frac{\overset{\circ}{\mu}}{RT}(\text{Am}^{3+}) - \frac{\overset{\circ}{\mu}}{RT}(\text{Pu}^{3+}) \right) \quad (1)$$

or

$$\frac{\overset{\circ}{\mu}}{RT}(\text{Pu(III) Species}) = \frac{\overset{\circ}{\mu}}{RT}(\text{Am(III) Species}) + v 8.294 \quad (2)$$

where v is the stoichiometric coefficient of Pu(III) and Am(III) in the species. The related equations between Am(III) and Nd(III) species are

$$\frac{\overset{\circ}{\mu}}{RT}(\text{Am(III) Species}) = \frac{\overset{\circ}{\mu}}{RT}(\text{Nd(III) Species}) - v \left(\frac{\overset{\circ}{\mu}}{RT}(\text{Nd}^{3+}) - \frac{\overset{\circ}{\mu}}{RT}(\text{Am}^{3+}) \right) \quad (3)$$

or

$$\frac{\overset{\circ}{\mu}}{RT}(\text{Am(III) Species}) = \frac{\overset{\circ}{\mu}}{RT}(\text{Nd(III) Species}) + v 29.232 \quad (4)$$

where $\frac{\overset{\circ}{\mu}}{RT}(\text{Nd}^{3+}) = -270.926$ (Rao et al., 1996).

The binary interaction parameters values used for $\text{Am}^{3+}\text{-Cl}^-$ 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 $\text{Pu}(\text{OH})_3(\text{s})$. 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).

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Appendix V: Memorandum on Current Release of Data Base

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Appendix V: Memorandum on Current Release of Data Base

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Appendix V: Memorandum on Current Release of Data Base

Table 1. Dimensionless standard chemical potentials for Am(III) and Pu(III) species.

Species	$\frac{\circ}{RT} \mu$	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 ·6H ₂ O(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

Appendix V: Memorandum on Current Release of Data Base

Species	$\frac{\Delta G_f^\circ}{RT}$	Source
PuOH_2^+	-307.058	Appendix A
Pu(OH)_2^+	-383.987	Appendix A
$\text{Pu(OH)}_3(\text{aq})$	-463.309	Appendix A
$\text{PuOHCO}_3(\text{s})$	-561.686	Felmy et al., 1990
$\text{Pu(OH)}_3(\text{s})$	-484.000	Felmy et al., 1989
$\text{NaPu(CO}_3)_2 \cdot 6\text{H}_2\text{O}(\text{c})$	-1388.174	Rao et al., 1996
$\text{PuPO}_4(\text{c})$	-701.456	Rai et al., 1992

Appendix V: Memorandum on Current Release of Data Base

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 ₂ PO 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

Appendix V: Memorandum on Current Release of Data Base

Table 3. Dimensionless standard chemical potentials for Th(IV) species.

Species	$\frac{\circ}{RT}$	Source
Th ⁴⁺	-284.227	Felmy et al., 1991
Th(CO ₃) ₅ ⁶⁻	-1411.378 [@]	Felmy et al., 1996
Th(OH) ₃ CO 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 •9H ₂ O(s)	-1775.90	Felmy and Rai, 1992
Th(SO ₄) ₂ •8H ₂ O(s)	-1680.00	Felmy and Rai, 1992
Th(SO ₄) ₂ •Na ₂ SO ₄ •6H ₂ O(s, 16_C)	-2011.29	Felmy and Rai, 1992
Th(SO ₄) ₂ •K ₂ SO ₄ •4H ₂ O(s, 16_C)	-1837.57	Felmy and Rai, 1992
Th(SO ₄) ₂ •2K ₂ SO ₄ •2H ₂ O(s, 16_C)	-2181.81	Felmy and Rai, 1992
Th(SO ₄) ₂ •3.5K ₂ SO 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

Appendix V: Memorandum on Current Release of Data Base

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

Appendix V: Memorandum on Current Release of Data Base

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	$\frac{\Delta G^\circ}{RT}$	Source
NpO_2^+	-369.109	Fuger and Oetting, 1976
$\text{NpO}_2\text{CO}_3^-$	-593.635	Fanghänel et al., 1995
$\text{NpO}_2(\text{CO}_3)_2^{3-}$	-809.895	Fanghänel et al., 1995
$\text{NpO}_2(\text{CO}_3)_3^{5-}$	-1020.306	Fanghänel et al., 1995
$\text{NpO}_2\text{OH}(\text{aq})$	-438.738	Fanghänel et al., 1995
$\text{NpO}_2(\text{OH})_2^-$	-506.249	Fanghänel et al., 1995
$\text{NaNpO}_2\text{CO}_3(\text{s})$	-712.871	Fanghänel et al., 1995
$\text{NaNpO}_2\text{CO}_3 \cdot 3.5\text{H}_2\text{O}(\text{s})$	-1048.062	Fanghänel et al., 1995
$\text{Na}_3\text{NpO}_2(\text{CO}_3)_2(\text{s})$	-1144.601	Fanghänel et al., 1995
$\text{NpO}_2\text{OH}(\text{am})$	-452.761	Fanghänel et al., 1995
$\text{NpO}_2\text{OH}(\text{aged})$	-454.373	Fanghänel et al., 1995
$\text{KNpO}_2\text{CO}_3(\text{s})$	-727.33	Novak et al., 1996
$\text{K}_3\text{NpO}_2(\text{CO}_3)_2(\text{s})$	-1173.55	Novak et al., 1996

Appendix V: Memorandum on Current Release of Data Base

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^+	$\text{NpO}_2(\text{OH})_2^-$	0	0	0	0	Fanghänel et al., 1995
Na^+	$\text{NpO}_2\text{CO}_3^-$	0.10	0.34	0	0	Fanghänel et al., 1995
Na^+	$\text{NpO}_2(\text{CO}_3)_2^{3-}$	0.48	4.4	0	0	Fanghänel et al., 1995
Na^+	$\text{NpO}_2(\text{CO}_3)_3^{5-}$	1.80	22.7	0	0	Fanghänel et al., 1995
K^+	$\text{NpO}_2\text{CO}_3^-$	0.10	0.34	0	0	Novak et al., 1996
K^+	$\text{NpO}_2(\text{CO}_3)_2^{3-}$	0.48	4.4	0	0	Novak et al., 1996
K^+	$\text{NpO}_2(\text{CO}_3)_3^{5-}$	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

Appendix V: Memorandum on Current Release of Data Base

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
$\text{NpO}_2(\text{OH})_2^-$	Cl^-	-	-0.24	-	Fanghänel et al., 1995
$\text{NpO}_2\text{CO}_3^-$	Cl^-	-	-0.21	-	Fanghänel et al., 1995
$\text{NpO}_2(\text{CO}_3)_2^{3-}$	Cl^-	-	-0.26	-	Fanghänel et al., 1995
$\text{NpO}_2(\text{CO}_3)_3^{5-}$	Cl^-	-	-0.26	-	Fanghänel et al., 1995
$\text{NpO}_2(\text{CO}_3)_3^{5-}$	CO_3^{2-}	-	-1.9	-	Novak et al., 1996

Neutral Interaction Parameters

n	i	λ_{ni}	Source
$\text{NpO}_2\text{OH}(\text{aq})$	Na^+	0	Fanghänel et al., 1995
$\text{NpO}_2\text{OH}(\text{aq})$	Cl^-	-0.19	Fanghänel et al., 1995

Appendix V: Memorandum on Current Release of Data Base

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).

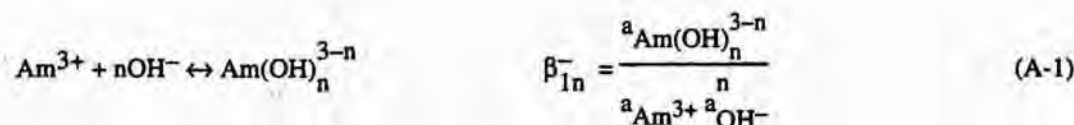
i	j	$\beta_{ij}^{(0)}$	$\beta_{ij}^{(1)}$	$\beta_{ij}^{(2)}$	Source
Na ⁺	CO ₃ ²⁻	0.0399	1.389	0.0044	Harvie et al., 1984
Na ⁺	CO ₃ ²⁻	0.0362	1.510	0.0052	Pitzer, 1991
Na ⁺	HCO ₃ ⁻	0.0277	0.0411	0	Harvie et al., 1984
Na ⁺	HCO ₃ ⁻	0.028	0.044	0	Pitzer, 1991

Appendix V: Memorandum on Current Release of Data Base

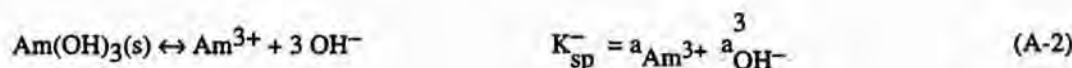
Appendix A: Parameter Values for +III Actinide Hydrolysis Species

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 $\text{Am(OH)}_3(\text{aq})$. 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



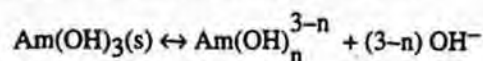
and the solubility of americium hydroxide is given by



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 $\text{Am(OH)}_3(\text{s})$ 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.,

Appendix V: Memorandum on Current Release of Data Base



$$\beta_{1n}^- K_{sp}^- = a_{\text{Am(OH)}_n^{3-n}} a_{\text{OH}^-}^{(3-n)} \quad (\text{A-3})$$

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 logK_{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 9.2×10⁻¹⁰M, or 1.03×10⁻⁹m 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 1×10⁻⁹m 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)

logβ ₁₁ ⁻	logβ ₁₂ ⁻	logβ ₁₃ ⁻	logK _{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

369	1	.3159	1.614	.0	-.00034	Ca++ C1-	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	-2.303	-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	1	.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---	
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	3	.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++ Oxx-	
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++ C1-	HMW84
424	2	.2210	3.143	-17.23	.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	2	.0	.0	.0	.0	Mg++ B3O3(OH)4-	FW86
431	1	.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---	
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	1	.0	.0	.0	.0	Mg++ Th(CO3)5---	
446	1	.0	.0	.0	.0	Mg++ HOx-	
447	2	.0	.0	.0	.0	Mg++ Oxx-	
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	1	.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	1	.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	1	.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+ C1-	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

617	1	.0	.0	.0	MgB(OH)4+ HEDTA--
618	1	.0	.0	.0	MgB(OH)4+ EDTA--
619	1	.0	.0	.0	MgB(OH)4+ AmEDTA--
620	1	.0	.0	.0	MgB(OH)4+ NpO2Cit-
621	1	.0	.0	.0	MgB(OH)4+ NpO2EDTA--
622	1	.0	.0	.0	MgB(OH)4+ NpO2Ox-
623	1	.0	.0	.0	MgB(OH)4+ U(OH)4(CO3)2--
624	1	.0	.0	.0	MgB(OH)4+ U(CO3)5---
625	1	.0	.0	.0	MgB(OH)4+ U(SO4)3-
626	1	.0	.0	.0	MgB(OH)4+ Pu(CO3)2-
627	1	.0	.0	.0	MgB(OH)4+ Pu(CO3)3--
628	1	.0	.0	.0	MgB(OH)4+ PuEDTA-
629	1	.0	.0	.0	MgB(OH)4+ CaCit-
630	1	.0	.0	.0	MgB(OH)4+ CaEDTA-
631	1	.0	.0	.0	MgB(OH)4+ UmuAn#2-
632	1	.0	.0	.0	MgB(OH)4+ UmuAn#3-
633	1	.0	.0	.0	MgB(OH)4+ UmuAn#4-
634	1	.0	.0	.0	MgB(OH)4+ U(OH)2(CO3)2-
635	1	.0	.0	.0	MgB(OH)4+ MgCit-
636	1	.0	.0	.0	MgB(OH)4+ MgEDTA-
637	1	.0	.0	.0	MgB(OH)4+ UmuAn#1-
638					
639	1	.12	.0	.0	CaB(OH)4+ Cl-
640	1	.0	.0	.0	CaB(OH)4+ SO4- HM#94
641	1	.0	.0	.0	CaB(OH)4+ HSO4- HM#84
642	1	.0	.0	.0	CaB(OH)4+ OH- HM#84
643	1	.0	.0	.0	CaB(OH)4+ HCO3- HM#94
644	1	.0	.0	.0	CaB(OH)4+ CO3- HM#94
645	1	.0	.0	.0	CaB(OH)4+ B(OH)4-
646	1	.0	.0	.0	CaB(OH)4+ B(O3)(OH)4-
647	1	.0	.0	.0	CaB(OH)4+ B(O5)(OH)4-
648	1	.0	.0	.0	CaB(OH)4+ Br-
649	1	.0	.0	.0	CaB(OH)4+ Am(CO3)2-
650	1	.0	.0	.0	CaB(OH)4+ Am(CO3)3--
651	1	.0	.0	.0	CaB(OH)4+ ClO4-
652	1	.0	.0	.0	CaB(OH)4+ NpO2(OH)2-
653	1	.0	.0	.0	CaB(OH)4+ NpO2CO3-
654	1	.0	.0	.0	CaB(OH)4+ NpO2(CO3)2--
655	1	.0	.0	.0	CaB(OH)4+ NpO2(CO3)3---
656	1	.0	.0	.0	CaB(OH)4+ H2PO4-
657	1	.0	.0	.0	CaB(OH)4+ HPO4-
658	1	.0	.0	.0	CaB(OH)4+ PO4--
659	1	.0	.0	.0	CaB(OH)4+ Th(SO4)3-
660	1	.0	.0	.0	CaB(OH)4+ Th(OH)3(CO3)-
661	1	.0	.0	.0	CaB(OH)4+ Th(CO3)5---
662	1	.0	.0	.0	CaB(OH)4+ H2Ox-
663	1	.0	.0	.0	CaB(OH)4+ Oxs-
664	1	.0	.0	.0	CaB(OH)4+ Ac-
665	1	.0	.0	.0	CaB(OH)4+ Lac-
666	1	.0	.0	.0	CaB(OH)4+ HClit-
667	1	.0	.0	.0	CaB(OH)4+ HClit-
668	1	.0	.0	.0	CaB(OH)4+ Cit-
669	1	.0	.0	.0	CaB(OH)4+ H3EDTA-
670	1	.0	.0	.0	CaB(OH)4+ H2EDTA-
671	1	.0	.0	.0	CaB(OH)4+ HEDTA-
672	1	.0	.0	.0	CaB(OH)4+ EDTA--
673	1	.0	.0	.0	CaB(OH)4+ AmEDTA--
674	1	.0	.0	.0	CaB(OH)4+ NpO2Cit-
675	1	.0	.0	.0	CaB(OH)4+ NpO2EDTA--
676	1	.0	.0	.0	CaB(OH)4+ NpO2Ox-
677	1	.0	.0	.0	CaB(OH)4+ U(OH)4(CO3)2--
678	1	.0	.0	.0	CaB(OH)4+ U(CO3)5---
679	1	.0	.0	.0	CaB(OH)4+ U(SO4)3-
680	1	.0	.0	.0	CaB(OH)4+ Pu(CO3)2-
681	1	.0	.0	.0	CaB(OH)4+ Pu(CO3)3--
682	1	.0	.0	.0	CaB(OH)4+ PuEDTA-
683	1	.0	.0	.0	CaB(OH)4+ CaCit-
684	1	.0	.0	.0	CaB(OH)4+ CaEDTA-
685	1	.0	.0	.0	CaB(OH)4+ UmuAn#2-
686	1	.0	.0	.0	CaB(OH)4+ UmuAn#3-
687	1	.0	.0	.0	CaB(OH)4+ UmuAn#4-
688	1	.0	.0	.0	CaB(OH)4+ U(OH)2(CO3)2-
689	1	.0	.0	.0	CaB(OH)4+ MgCit-
690	1	.0	.0	.0	CaB(OH)4+ MgEDTA-
691	1	.0	.0	.0	CaB(OH)4+ UmuAn#1-
692					
693	1	.6117	5.403	-0.0284	Am+++ Cl- FRFR89 (from HSC13 values)
694	3	3.0398	.0	-2500	Am+++ SO4- RPF94
695	1	.0	.0	.0	Am+++ HSO4-
696	1	.0	.0	.0	Am+++ OH-
697	1	.0	.0	.0	Am+++ HCO3-
698	3	.0	.0	.0	Am+++ CO3-
699	1	.0	.0	.0	Am+++ B(OH)4-
700	1	.0	.0	.0	Am+++ B(O3)(OH)4-
701	3	.0	.0	.0	Am+++ B(O5)(OH)4-
702	1	.0	.0	.0	Am+++ Br-
703	1	.0	.0	.0	Am+++ Am(CO3)2-
704	3	.0	.0	.0	Am+++ Am(CO3)3--
705	1	.80	5.35	-0.0048	Am+++ ClO4- FRF90
706	1	.0	.0	.0	Am+++ NpO2(OH)2-
707	1	.0	.0	.0	Am+++ NpO2CO3-
708	3	.0	.0	.0	Am+++ NpO2(CO3)2--
709	3	.0	.0	.0	Am+++ NpO2(CO3)3---
710	1	.0	.0	.0	Am+++ H2PO4- RPF94 (from H2-H2PO4 value)
711	3	.0	.0	.0	Am+++ HPO4-
712	3	.0	.0	.0	Am+++ PO4--
713	3	.0	.0	.0	Am+++ Th(SO4)3-
714	1	.0	.0	.0	Am+++ Th(OH)3(CO3)-
715	3	.0	.0	.0	Am+++ Th(CO3)5---
716	1	.0	.0	.0	Am+++ H2Ox-
717	3	.0	.0	.0	Am+++ Oxs-
718	1	.0	.0	.0	Am+++ Ac-
719	1	.0	.0	.0	Am+++ Lac-
720	1	.0	.0	.0	Am+++ HClit-
721	3	.0	.0	.0	Am+++ HClit-
722	3	.0	.0	.0	Am+++ Cit-
723	3	.0	.0	.0	Am+++ H3EDTA-
724	3	.0	.0	.0	Am+++ H2EDTA-
725	3	.0	.0	.0	Am+++ HEDTA-
726	3	.0	.0	.0	Am+++ EDTA--
727	3	.0	.0	.0	Am+++ AmEDTA--
728	3	.0	.0	.0	Am+++ NpO2Cit-
729	3	.0	.0	.0	Am+++ NpO2EDTA--
730	1	.0	.0	.0	Am+++ NpO2Ox-
731	3	.0	.0	.0	Am+++ U(OH)4(CO3)2--
732	3	.0	.0	.0	Am+++ U(CO3)5---
733	3	.0	.0	.0	Am+++ U(SO4)3-
734	1	.0	.0	.0	Am+++ Pu(CO3)2-
735	1	.0	.0	.0	Am+++ Pu(CO3)3--
736	1	.0	.0	.0	Am+++ PuEDTA-
737	1	.0	.0	.0	Am+++ CaCit-
738	3	.0	.0	.0	Am+++ CaEDTA-
739	3	.0	.0	.0	Am+++ UmuAn#2-
740	1	.0	.0	.0	Am+++ UmuAn#3-

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

741	3	.0	.0	.0	.0	Am+++ UmuAn#4-
742	3	.0	.0	.0	.0	Am+++ U(OH)2(CO3)2-
743	1	.0	.0	.0	.0	Am+++ MgCl-
744	3	.0	.0	.0	.0	Am+++ MgEDTA-
745	1	.0	.0	.0	.0	Am+++ UmuAn#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+ NO3-
771	1	.0	.0	.0	.0	AmCO3+ Oxo-
772	1	.0	.0	.0	.0	AmCO3+ Ac-
773	1	.0	.0	.0	.0	AmCO3+ Lac-
774	1	.0	.0	.0	.0	AmCO3+ H2C1t-
775	1	.0	.0	.0	.0	AmCO3+ HC1t-
776	1	.0	.0	.0	.0	AmCO3+ Clt--
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+ NpO2C1t-
783	1	.0	.0	.0	.0	AmCO3+ NpO2EDTA---
784	1	.0	.0	.0	.0	AmCO3+ NpO2Oxo-
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+ CaClt-
792	1	.0	.0	.0	.0	AmCO3+ CaEDTA-
793	1	.0	.0	.0	.0	AmCO3+ UmuAn#2-
794	1	.0	.0	.0	.0	AmCO3+ UmuAn#3-
795	1	.0	.0	.0	.0	AmCO3+ UmuAn#4-
796	1	.0	.0	.0	.0	AmCO3+ U(OH)2(CO3)2-
797	1	.0	.0	.0	.0	AmCO3+ MgCl-
798	1	.0	.0	.0	.0	AmCO3+ MgEDTA-
799	1	.0	.0	.0	.0	AmCO3+ UmuAn#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	1.16	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	1	.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	1	.0	.0	.0	.0	Th++++ NO3-
825	1	.0	.0	.0	.0	Th++++ Oxo-
826	1	.0	.0	.0	.0	Th++++ Ac-
827	1	.0	.0	.0	.0	Th++++ Lac-
828	1	.0	.0	.0	.0	Th++++ H2C1t-
829	1	.0	.0	.0	.0	Th++++ HC1t-
830	3	.0	.0	.0	.0	Th++++ Clt--
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++++ NpO2C1t-
837	3	.0	.0	.0	.0	Th++++ NpO2EDTA---
838	1	.0	.0	.0	.0	Th++++ NpO2Oxo-
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++++ CaClt-
846	3	.0	.0	.0	.0	Th++++ CaEDTA-
847	3	.0	.0	.0	.0	Th++++ UmuAn#2-
848	1	.0	.0	.0	.0	Th++++ UmuAn#3-
849	3	.0	.0	.0	.0	Th++++ UmuAn#4-
850	3	.0	.0	.0	.0	Th++++ U(OH)2(CO3)2-
851	1	.0	.0	.0	.0	Th++++ MgCl-
852	3	.0	.0	.0	.0	Th++++ MgEDTA-
853	1	.0	.0	.0	.0	Th++++ UmuAn#1-
854						
855	1	.6117	5.403	.0	-.0284	Pu++++ Cl- FRSR89 (from MIC13 values)
856	3	3.0398	.0	-2500	.0	Pu++++ SO4- RPT94
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	1	.0	.0	.0	.0	Pu+++ Pu(CO3)3=	
867	1	1.80	5.35	-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	1	.0	.0	.0	.0	Pu+++ NpO2(CO3)3=	
872	1	.0	.0	.0	.0	Pu+++ H2PO4-	RFF94 (from Nd-H2PO4 value)
873	1	.0	.0	.0	.0	Pu+++ HPO4=	
874	1	.0	.0	.0	.0	Pu+++ PO4=	
875	1	.0	.0	.0	.0	Pu+++ Th(SO4)3=	
876	1	.0	.0	.0	.0	Pu+++ Th(OH)3(CO3)-	
877	1	.0	.0	.0	.0	Pu+++ Th(CO3)5=	
878	1	.0	.0	.0	.0	Pu+++ Hox-	
879	1	.0	.0	.0	.0	Pu+++ Oxe-	
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	1	.0	.0	.0	.0	Pu+++ HCit-	
884	1	.0	.0	.0	.0	Pu+++ Cit-	
885	1	.0	.0	.0	.0	Pu+++ H3EDTA-	
886	1	.0	.0	.0	.0	Pu+++ H2EDTA-	
887	1	.0	.0	.0	.0	Pu+++ HEDTA=	
888	1	.0	.0	.0	.0	Pu+++ EDTA=	
889	1	.0	.0	.0	.0	Pu+++ PuEDTA=	
890	1	.0	.0	.0	.0	Pu+++ NpO2Cit-	
891	1	.0	.0	.0	.0	Pu+++ NpO2EDTA=	
892	1	.0	.0	.0	.0	Pu+++ NpO2Ox-	
893	1	.0	.0	.0	.0	Pu+++ U(OH)4(CO3)2=	
894	1	.0	.0	.0	.0	Pu+++ U(CO3)5=	
895	1	.0	.0	.0	.0	Pu+++ U(SO4)3=	
896	1	.0	.0	.0	.0	Pu+++ Pu(CO3)2-	
897	1	.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	1	.0	.0	.0	.0	Pu+++ CaEDTA=	
901	1	.0	.0	.0	.0	Pu+++ UmuAn#2-	
902	1	.0	.0	.0	.0	Pu+++ UmuAn#3-	
903	1	.0	.0	.0	.0	Pu+++ UmuAn#4-	
904	1	.0	.0	.0	.0	Pu+++ U(OH)2(CO3)2=	
905	1	.0	.0	.0	.0	Pu+++ MgCit-	
906	1	.0	.0	.0	.0	Pu+++ MgEDTA=	
907	1	.0	.0	.0	.0	Pu+++ UmuAn#1-	
908	1	1.1415	.281	.0	.0	NpO2- Cl-	NFRK95
909	1	.0	.0	.0	.0	NpO2- SO4=	
910	1	.0	.0	.0	.0	NpO2- HSO4-	
911	1	.0	.0	.0	.0	NpO2- OH-	
912	1	.0	.0	.0	.0	NpO2- HCO3-	
913	1	.0	.0	.0	.0	NpO2- CO3=	
914	1	.0	.0	.0	.0	NpO2- B(OH)4-	
915	1	.0	.0	.0	.0	NpO2- B(OH)3(OH)4-	
916	1	.0	.0	.0	.0	NpO2- B(OH)4(OH)4-	
917	1	.0	.0	.0	.0	NpO2- Br-	
918	1	.0	.0	.0	.0	NpO2- Am(CO3)2-	
919	1	.0	.0	.0	.0	NpO2- Am(CO3)3=	
920	1	.0	.0	.0	.0	NpO2- ClO4-	NFRK95
921	1	.257	.180	.0081		NpO2- NpO2(OH)2-	
922	1	.0	.0	.0	.0	NpO2- NpO2CO3-	
923	1	.0	.0	.0	.0	NpO2- NpO2(CO3)2=	
924	1	.0	.0	.0	.0	NpO2- NpO2(CO3)3=	
925	1	.0	.0	.0	.0	NpO2- K2PO4-	
926	1	.0	.0	.0	.0	NpO2- HPO4=	
927	1	.0	.0	.0	.0	NpO2- PO4=	
928	1	.0	.0	.0	.0	NpO2- Th(SO4)3=	
929	1	.0	.0	.0	.0	NpO2- Th(OH)3(CO3)-	
930	1	.0	.0	.0	.0	NpO2- Th(CO3)5=	
931	1	.0	.0	.0	.0	NpO2- Hox-	
932	1	.0	.0	.0	.0	NpO2- Oxe-	
933	1	.0	.0	.0	.0	NpO2- Ac-	
934	1	.0	.0	.0	.0	NpO2- Lac-	
935	1	.0	.0	.0	.0	NpO2- H2Cit-	
936	1	.0	.0	.0	.0	NpO2- HCit-	
937	1	.0	.0	.0	.0	NpO2- Cit-	
938	1	.0	.0	.0	.0	NpO2- H3EDTA-	
939	1	.0	.0	.0	.0	NpO2- H2EDTA-	
940	1	.0	.0	.0	.0	NpO2- HEDTA=	
941	1	.0	.0	.0	.0	NpO2- EDTA=	
942	1	.0	.0	.0	.0	NpO2- AmEDTA=	
943	1	.0	.0	.0	.0	NpO2- NpO2Cit-	
944	1	.0	.0	.0	.0	NpO2- NpO2EDTA=	
945	1	.0	.0	.0	.0	NpO2- NpO2Ox-	
946	1	.0	.0	.0	.0	NpO2- U(OH)4(CO3)2=	
947	1	.0	.0	.0	.0	NpO2- U(CO3)5=	
948	1	.0	.0	.0	.0	NpO2- U(SO4)3=	
949	1	.0	.0	.0	.0	NpO2- Pu(CO3)2-	
950	1	.0	.0	.0	.0	NpO2- Pu(CO3)3=	
951	1	.0	.0	.0	.0	NpO2- PuEDTA-	
952	1	.0	.0	.0	.0	NpO2- CaCit-	
953	1	.0	.0	.0	.0	NpO2- CaEDTA=	
954	1	.0	.0	.0	.0	NpO2- UmuAn#2-	
955	1	.0	.0	.0	.0	NpO2- UmuAn#3-	
956	1	.0	.0	.0	.0	NpO2- UmuAn#4-	
957	1	.0	.0	.0	.0	NpO2- U(OH)2(CO3)2=	
958	1	.0	.0	.0	.0	NpO2- MgCit-	
959	1	.0	.0	.0	.0	NpO2- MgEDTA=	
960	1	.0	.0	.0	.0	NpO2- UmuAn#1-	
961	1	.0	.0	.0	.0		
962	1	1.644	15.5	.0	.1	U++++ Cl-	RFS000
963	1	.0	.0	.0	.0	U++++ SO4=	
964	1	.0	.0	.0	.0	U++++ HSO4-	
965	1	.0	.0	.0	.0	U++++ OH-	
966	1	.0	.0	.0	.0	U++++ HCO3-	
967	1	.0	.0	.0	.0	U++++ CO3=	
968	1	.0	.0	.0	.0	U++++ B(OH)4-	
969	1	.0	.0	.0	.0	U++++ B(OH)3(OH)4-	
970	1	.0	.0	.0	.0	U++++ B(OH)4(OH)4-	
971	1	.0	.0	.0	.0	U++++ Br-	
972	1	.0	.0	.0	.0	U++++ Am(CO3)2-	
973	1	.0	.0	.0	.0	U++++ Am(CO3)3=	
974	1	.0	.0	.0	.0	U++++ ClO4-	
975	1	.0	.0	.0	.0	U++++ NpO2(OH)2-	
976	1	.0	.0	.0	.0	U++++ NpO2CO3-	
977	1	.0	.0	.0	.0	U++++ NpO2(CO3)2=	
978	1	.0	.0	.0	.0	U++++ NpO2(CO3)3=	
979	1	.0	.0	.0	.0	U++++ K2PO4-	
980	1	.0	.0	.0	.0	U++++ HPO4=	
981	1	.0	.0	.0	.0	U++++ PO4=	
982	1	.0	.0	.0	.0	U++++ Th(SO4)3=	
983	1	.0	.0	.0	.0	U++++ Th(OH)3(CO3)-	
984	1	.0	.0	.0	.0	U++++ Th(CO3)5=	
985	1	.0	.0	.0	.0	U++++ Hox-	
986	1	.0	.0	.0	.0	U++++ Oxe-	
987	1	.0	.0	.0	.0	U++++ Ac-	
988	1	.0	.0	.0	.0		

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

898	1	.0	.0	.0	.0	U**** Lac-	
899	1	.0	.0	.0	.0	U**** H2Cl1-	
900	3	.0	.0	.0	.0	U**** HCl1-	
901	3	.0	.0	.0	.0	U**** Cl1-	
902	1	.0	.0	.0	.0	U**** H3EDTA-	
903	1	.0	.0	.0	.0	U**** H2EDTA-	
904	3	.0	.0	.0	.0	U**** HEDTA--	
905	3	.0	.0	.0	.0	U**** EDTA--	
906	3	.0	.0	.0	.0	U**** AmEDTA--	
907	3	.0	.0	.0	.0	U**** NpO2Cl1-	
908	3	.0	.0	.0	.0	U**** NpO2EDTA--	
909	3	.0	.0	.0	.0	U**** NpO2Ox-	
910	1	.0	.0	.0	.0	U**** U(OH)4(CO3)2==	
911	3	.0	.0	.0	.0	U**** U(CO3)5===	
912	3	.0	.0	.0	.0	U**** U(SO4)3=	
913	1	.0	.0	.0	.0	U**** Pu(CO3)2-	
914	3	.0	.0	.0	.0	U**** Pu(CO3)3--	
915	1	.0	.0	.0	.0	U**** PuEDTA-	
916	1	.0	.0	.0	.0	U**** CaCl1-	
917	3	.0	.0	.0	.0	U**** CaEDTA-	
918	3	.0	.0	.0	.0	U**** UruAn#2-	
919	1	.0	.0	.0	.0	U**** UruAn#3-	
920	1	.0	.0	.0	.0	U**** UruAn#4-	
921	3	.0	.0	.0	.0	U**** U(OH)2(CO3)2-	
922	1	.0	.0	.0	.0	U**** MgCl1-	
923	3	.0	.0	.0	.0	U**** MgEDTA-	
924	1	.0	.0	.0	.0	U**** UruAn#1-	
925	1	1.0	7.856	.0	.0	DOH*** Cl-	2F000
926	3	.0	.0	.0	.0	DOH*** SO4-	
927	1	.0	.0	.0	.0	DOH*** HSO4-	
928	1	.0	.0	.0	.0	DOH*** OH-	
929	1	.0	.0	.0	.0	DOH*** HCO3-	
930	3	.0	.0	.0	.0	DOH*** CO3=	
931	1	.0	.0	.0	.0	DOH*** B(OH)4-	
932	1	.0	.0	.0	.0	DOH*** B3O3(OH)4-	
933	3	.0	.0	.0	.0	DOH*** B4O5(OH)4-	
934	1	.0	.0	.0	.0	DOH*** Br-	
935	1	.0	.0	.0	.0	DOH*** Am(CO3)2-	
936	3	.0	.0	.0	.0	DOH*** Am(CO3)3--	
937	1	.0	.0	.0	.0	DOH*** ClO4-	
938	1	.0	.0	.0	.0	DOH*** NpO2(OH)2-	
939	1	.0	.0	.0	.0	DOH*** NpO2CO3-	
940	3	.0	.0	.0	.0	DOH*** NpO2(CO3)2--	
941	3	.0	.0	.0	.0	DOH*** NpO2(CO3)3---	
942	3	.0	.0	.0	.0	DOH*** H2PO4-	
943	3	.0	.0	.0	.0	DOH*** HPO4-	
944	3	.0	.0	.0	.0	DOH*** PO4--	
945	3	.0	.0	.0	.0	DOH*** Th(SO4)3=	
946	1	.0	.0	.0	.0	DOH*** Th(OH)3(CO3)-	
947	3	.0	.0	.0	.0	DOH*** Th(CO3)5===	
948	1	.0	.0	.0	.0	DOH*** HCl-	
949	1	.0	.0	.0	.0	DOH*** Ox-	
950	1	.0	.0	.0	.0	DOH*** Ac-	
951	1	.0	.0	.0	.0	DOH*** Lac-	
952	1	.0	.0	.0	.0	DOH*** H2Cl1-	
953	3	.0	.0	.0	.0	DOH*** HCl1-	
954	3	.0	.0	.0	.0	DOH*** Cl1-	
955	1	.0	.0	.0	.0	DOH*** H3EDTA-	
956	1	.0	.0	.0	.0	DOH*** H2EDTA-	
957	3	.0	.0	.0	.0	DOH*** HEDTA--	
958	3	.0	.0	.0	.0	DOH*** EDTA--	
959	3	.0	.0	.0	.0	DOH*** AmEDTA--	
960	3	.0	.0	.0	.0	DOH*** NpO2Cl1-	
961	3	.0	.0	.0	.0	DOH*** NpO2EDTA--	
962	3	.0	.0	.0	.0	DOH*** NpO2Ox-	
963	3	.0	.0	.0	.0	DOH*** U(OH)4(CO3)2==	
964	3	.0	.0	.0	.0	DOH*** U(CO3)5===	
965	3	.0	.0	.0	.0	DOH*** U(SO4)3=	
966	1	.0	.0	.0	.0	DOH*** Pu(CO3)2-	
967	3	.0	.0	.0	.0	DOH*** Pu(CO3)3--	
968	1	.0	.0	.0	.0	DOH*** PuEDTA-	
969	3	.0	.0	.0	.0	DOH*** CaCl1-	
970	3	.0	.0	.0	.0	DOH*** CaEDTA-	
971	3	.0	.0	.0	.0	DOH*** UruAn#2-	
972	1	.0	.0	.0	.0	DOH*** UruAn#3-	
973	3	.0	.0	.0	.0	DOH*** UruAn#4-	
974	3	.0	.0	.0	.0	DOH*** U(OH)2(CO3)2-	
975	3	.0	.0	.0	.0	DOH*** MgCl1-	
976	3	.0	.0	.0	.0	DOH*** MgEDTA-	
977	1	.0	.0	.0	.0	DOH*** UruAn#1-	
978	1	1.239	4.934	.0	.0	UAc*** Cl-	analogy w/ThAc***
979	3	.0	.0	.0	.0	UAc*** SO4-	
980	1	.0	.0	.0	.0	UAc*** HSO4-	
981	1	.0	.0	.0	.0	UAc*** OH-	
982	1	.0	.0	.0	.0	UAc*** HCO3-	
983	3	.0	.0	.0	.0	UAc*** CO3=	
984	1	.0	.0	.0	.0	UAc*** B(OH)4-	
985	1	.0	.0	.0	.0	UAc*** B3O3(OH)4-	
986	3	.0	.0	.0	.0	UAc*** B4O5(OH)4-	
987	1	.0	.0	.0	.0	UAc*** Br-	
988	3	.0	.0	.0	.0	UAc*** Am(CO3)2-	
989	1	.0	.0	.0	.0	UAc*** Am(CO3)3--	
990	1	.0	.0	.0	.0	UAc*** ClO4-	
991	1	.0	.0	.0	.0	UAc*** NpO2(OH)2-	
992	3	.0	.0	.0	.0	UAc*** NpO2CO3-	
993	3	.0	.0	.0	.0	UAc*** NpO2(CO3)2--	
994	3	.0	.0	.0	.0	UAc*** NpO2(CO3)3---	
995	3	.0	.0	.0	.0	UAc*** H2PO4-	
996	3	.0	.0	.0	.0	UAc*** HPO4-	
997	3	.0	.0	.0	.0	UAc*** PO4--	
998	3	.0	.0	.0	.0	UAc*** Th(SO4)3=	
999	1	.0	.0	.0	.0	UAc*** Th(OH)3(CO3)-	
1000	3	.0	.0	.0	.0	UAc*** Th(CO3)5===	
1001	1	.0	.0	.0	.0	UAc*** HCl-	
1002	1	.0	.0	.0	.0	UAc*** Ox-	
1003	1	.0	.0	.0	.0	UAc*** Ac-	
1004	1	.0	.0	.0	.0	UAc*** Lac-	
1005	1	.0	.0	.0	.0	UAc*** H2Cl1-	
1006	3	.0	.0	.0	.0	UAc*** HCl1-	
1007	3	.0	.0	.0	.0	UAc*** Cl1-	
1008	1	.0	.0	.0	.0	UAc*** H3EDTA-	
1009	1	.0	.0	.0	.0	UAc*** H2EDTA-	
1010	3	.0	.0	.0	.0	UAc*** HEDTA--	
1011	3	.0	.0	.0	.0	UAc*** EDTA--	
1012	3	.0	.0	.0	.0	UAc*** AmEDTA--	
1013	3	.0	.0	.0	.0	UAc*** NpO2Cl1-	
1014	3	.0	.0	.0	.0	UAc*** NpO2EDTA--	
1015	3	.0	.0	.0	.0	UAc*** NpO2Ox-	
1016	3	.0	.0	.0	.0	UAc*** U(OH)4(CO3)2==	
1017	3	.0	.0	.0	.0	UAc*** U(CO3)5===	
1018	3	.0	.0	.0	.0	UAc*** U(SO4)3=	
1019	1	.0	.0	.0	.0	UAc*** Pu(CO3)2-	
1020	3	.0	.0	.0	.0	UAc*** Pu(CO3)3--	

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

1113	3	.0	.0	.0	UAc+++ Pu(CO3)3--
1114	1	.0	.0	.0	UAc+++ PuEDTA-
1115	1	.0	.0	.0	UAc+++ CaC1C-
1116	3	.0	.0	.0	UAc+++ CaEDTA-
1117	3	.0	.0	.0	UAc+++ UmuAn#2-
1118	1	.0	.0	.0	UAc+++ UmuAn#3-
1119	3	.0	.0	.0	UAc+++ UmuAn#4-
1120	3	.0	.0	.0	UAc+++ U(OH)2(CO3)2-
1121	1	.0	.0	.0	UAc+++ MgC1C-
1122	3	.0	.0	.0	UAc+++ MgEDTA-
1123	1	.0	.0	.0	UAc+++ UmuAn#1-
1125	1	-2061	-.525	.0	ThOx++ C1-
1126	2	.0	.0	.0	ThOx++ SO4-
1127	1	.0	.0	.0	ThOx++ HSO4-
1128	1	.0	.0	.0	ThOx++ OH-
1129	1	.0	.0	.0	ThOx++ HCO3-
1130	2	.0	.0	.0	ThOx++ CO3-
1131	1	.0	.0	.0	ThOx++ B(OH)4-
1132	1	.0	.0	.0	ThOx++ B(OH)3(OH)4-
1133	2	.0	.0	.0	ThOx++ B(OH)3(OH)4-
1134	1	.0	.0	.0	ThOx++ Br-
1135	1	.0	.0	.0	ThOx++ Am(CO3)2-
1136	3	.0	.0	.0	ThOx++ Am(CO3)3--
1137	1	.0	.0	.0	ThOx++ C1O4-
1138	1	.0	.0	.0	ThOx++ NpO2(OH)2-
1139	1	.0	.0	.0	ThOx++ NpO2CO3-
1140	3	.0	.0	.0	ThOx++ NpO2(CO3)2--
1141	3	.0	.0	.0	ThOx++ NpO2(CO3)3---
1142	1	.0	.0	.0	ThOx++ H2PO4-
1143	2	.0	.0	.0	ThOx++ HPO4-
1144	3	.0	.0	.0	ThOx++ PO4--
1145	2	.0	.0	.0	ThOx++ Th(SO4)3-
1146	1	.0	.0	.0	ThOx++ Th(OH)3(CO3)-
1147	3	.0	.0	.0	ThOx++ Th(CO3)5---
1148	1	.0	.0	.0	ThOx++ HOx-
1149	3	.0	.0	.0	ThOx++ Ox-
1150	1	.0	.0	.0	ThOx++ Ac-
1151	1	.0	.0	.0	ThOx++ Lac-
1152	1	.0	.0	.0	ThOx++ H2C1C-
1153	2	.0	.0	.0	ThOx++ HC1C-
1154	3	.0	.0	.0	ThOx++ C1C--
1155	3	.0	.0	.0	ThOx++ H3EDTA-
1156	3	.0	.0	.0	ThOx++ H2EDTA-
1157	3	.0	.0	.0	ThOx++ HEDTA--
1158	3	.0	.0	.0	ThOx++ EDTA--
1159	3	.0	.0	.0	ThOx++ AmEDTA--
1160	2	.0	.0	.0	ThOx++ NpO2C1C-
1161	3	.0	.0	.0	ThOx++ NpO2EDTA---
1162	1	.0	.0	.0	ThOx++ NpO2Ox-
1163	3	.0	.0	.0	ThOx++ U(OH)4(CO3)2--
1164	3	.0	.0	.0	ThOx++ U(CO3)5---
1165	2	.0	.0	.0	ThOx++ U(SO4)3-
1166	1	.0	.0	.0	ThOx++ Pu(CO3)2-
1167	2	.0	.0	.0	ThOx++ Pu(CO3)3--
1168	1	.0	.0	.0	ThOx++ PuEDTA-
1169	1	.0	.0	.0	ThOx++ CaC1C-
1170	2	.0	.0	.0	ThOx++ CaEDTA-
1171	3	.0	.0	.0	ThOx++ UmuAn#2-
1172	1	.0	.0	.0	ThOx++ UmuAn#3-
1173	2	.0	.0	.0	ThOx++ UmuAn#4-
1174	2	.0	.0	.0	ThOx++ U(OH)2(CO3)2-
1175	1	.0	.0	.0	ThOx++ MgC1C-
1176	2	.0	.0	.0	ThOx++ MgEDTA-
1177	1	.0	.0	.0	ThOx++ UmuAn#1-
1178	1	.0	.0	.0	ThOx++ UmuAn#1-
1179	1	-227	2.154	-.102	AmAc++ C1-
1180	2	.0	.0	.0	AmAc++ SO4-
1181	1	.0	.0	.0	AmAc++ HSO4-
1182	1	.0	.0	.0	AmAc++ OH-
1183	1	.0	.0	.0	AmAc++ HCO3-
1184	2	.0	.0	.0	AmAc++ CO3-
1185	1	.0	.0	.0	AmAc++ B(OH)4-
1186	1	.0	.0	.0	AmAc++ B(OH)3(OH)4-
1187	2	.0	.0	.0	AmAc++ B(OH)3(OH)4-
1188	1	.0	.0	.0	AmAc++ Br-
1189	1	.0	.0	.0	AmAc++ Am(CO3)2-
1190	3	.0	.0	.0	AmAc++ Am(CO3)3--
1191	1	.0	.0	.0	AmAc++ C1O4-
1192	1	.0	.0	.0	AmAc++ NpO2(OH)2-
1193	1	.0	.0	.0	AmAc++ NpO2CO3-
1194	3	.0	.0	.0	AmAc++ NpO2(CO3)2--
1195	3	.0	.0	.0	AmAc++ NpO2(CO3)3---
1196	1	.0	.0	.0	AmAc++ H2PO4-
1197	2	.0	.0	.0	AmAc++ HPO4-
1198	3	.0	.0	.0	AmAc++ PO4--
1199	2	.0	.0	.0	AmAc++ Th(SO4)3-
1200	1	.0	.0	.0	AmAc++ Th(OH)3(CO3)-
1201	3	.0	.0	.0	AmAc++ Th(CO3)5---
1202	1	.0	.0	.0	AmAc++ HOx-
1203	2	.0	.0	.0	AmAc++ Ox-
1204	1	.0	.0	.0	AmAc++ Ac-
1205	1	.0	.0	.0	AmAc++ Lac-
1206	1	.0	.0	.0	AmAc++ H2C1C-
1207	2	.0	.0	.0	AmAc++ HC1C-
1208	3	.0	.0	.0	AmAc++ C1C--
1209	3	.0	.0	.0	AmAc++ H3EDTA-
1210	3	.0	.0	.0	AmAc++ H2EDTA-
1211	3	.0	.0	.0	AmAc++ HEDTA--
1212	3	.0	.0	.0	AmAc++ EDTA--
1213	3	.0	.0	.0	AmAc++ AmEDTA--
1214	2	.0	.0	.0	AmAc++ NpO2C1C-
1215	3	.0	.0	.0	AmAc++ NpO2EDTA---
1216	1	.0	.0	.0	AmAc++ NpO2Ox-
1217	3	.0	.0	.0	AmAc++ U(OH)4(CO3)2--
1218	3	.0	.0	.0	AmAc++ U(CO3)5---
1219	3	.0	.0	.0	AmAc++ U(SO4)3-
1220	1	.0	.0	.0	AmAc++ Pu(CO3)2-
1221	2	.0	.0	.0	AmAc++ Pu(CO3)3--
1222	1	.0	.0	.0	AmAc++ PuEDTA-
1223	1	.0	.0	.0	AmAc++ CaC1C-
1224	2	.0	.0	.0	AmAc++ CaEDTA-
1225	3	.0	.0	.0	AmAc++ UmuAn#2-
1226	1	.0	.0	.0	AmAc++ UmuAn#3-
1227	2	.0	.0	.0	AmAc++ UmuAn#4-
1228	2	.0	.0	.0	AmAc++ U(OH)2(CO3)2-
1229	1	.0	.0	.0	AmAc++ MgC1C-
1230	2	.0	.0	.0	AmAc++ MgEDTA-
1231	1	.0	.0	.0	AmAc++ UmuAn#1-
1232	1	.0	.0	.0	AmAc++ UmuAn#1-
1233	1	-0572	6.331	.0	AmLac++ C1-
1234	2	.0	.0	.0	AmLac++ SO4-
1235	1	.0	.0	.0	AmLac++ HSO4-
1236	1	.0	.0	.0	AmLac++ OH-

RCM96

RCM96

RCM96

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

1237	1	.0	.0	.0	.0	AmLac++ NCO3-
1238	1	.0	.0	.0	.0	AmLac++ CO3-
1239	1	.0	.0	.0	.0	AmLac++ B(OH)4-
1240	1	.0	.0	.0	.0	AmLac++ B(OH)4-
1241	2	.0	.0	.0	.0	AmLac++ B(OH)4-
1242	1	.0	.0	.0	.0	AmLac++ B(OH)4-
1243	1	.0	.0	.0	.0	AmLac++ Br-
1244	3	.0	.0	.0	.0	AmLac++ Am(CO3)2-
1245	1	.0	.0	.0	.0	AmLac++ Am(CO3)3--
1246	1	.0	.0	.0	.0	AmLac++ ClO4-
1247	1	.0	.0	.0	.0	AmLac++ NpO2(OH)2-
1248	3	.0	.0	.0	.0	AmLac++ NpO2CO3-
1249	3	.0	.0	.0	.0	AmLac++ NpO2(CO3)2--
1250	1	.0	.0	.0	.0	AmLac++ NpO2(CO3)3---
1251	2	.0	.0	.0	.0	AmLac++ H2PO4-
1252	3	.0	.0	.0	.0	AmLac++ HPO4-
1253	2	.0	.0	.0	.0	AmLac++ PO4--
1254	1	.0	.0	.0	.0	AmLac++ Th(SO4)3-
1255	3	.0	.0	.0	.0	AmLac++ Th(OH)3(CO3)-
1256	1	.0	.0	.0	.0	AmLac++ Th(CO3)5---
1257	2	.0	.0	.0	.0	AmLac++ HOx-
1258	1	.0	.0	.0	.0	AmLac++ OX-
1259	1	.0	.0	.0	.0	AmLac++ Ac-
1260	1	.0	.0	.0	.0	AmLac++ Lac-
1261	2	.0	.0	.0	.0	AmLac++ HCit-
1262	3	.0	.0	.0	.0	AmLac++ HCit-
1263	3	.0	.0	.0	.0	AmLac++ Cit-
1264	3	.0	.0	.0	.0	AmLac++ H3EDTA-
1265	3	.0	.0	.0	.0	AmLac++ H2EDTA-
1266	3	.0	.0	.0	.0	AmLac++ HEDTA--
1267	3	.0	.0	.0	.0	AmLac++ EDTA--
1268	2	.0	.0	.0	.0	AmLac++ AmEDTA--
1269	3	.0	.0	.0	.0	AmLac++ NpO2Cit-
1270	1	.0	.0	.0	.0	AmLac++ NpO2EDTA---
1271	3	.0	.0	.0	.0	AmLac++ NpO2OX-
1272	3	.0	.0	.0	.0	AmLac++ U(OH)4(CO3)2--
1273	2	.0	.0	.0	.0	AmLac++ U(CO3)5---
1274	1	.0	.0	.0	.0	AmLac++ U(SO4)3-
1275	2	.0	.0	.0	.0	AmLac++ Pu(CO3)2-
1276	1	.0	.0	.0	.0	AmLac++ Pu(CO3)3--
1277	1	.0	.0	.0	.0	AmLac++ PuEDTA-
1278	2	.0	.0	.0	.0	AmLac++ CaCit-
1279	3	.0	.0	.0	.0	AmLac++ CaEDTA-
1280	1	.0	.0	.0	.0	AmLac++ UmuAn#2-
1281	2	.0	.0	.0	.0	AmLac++ UmuAn#3-
1282	2	.0	.0	.0	.0	AmLac++ UmuAn#4-
1283	1	.0	.0	.0	.0	AmLac++ U(OH)2(CO3)2-
1284	2	.0	.0	.0	.0	AmLac++ MgCit-
1285	1	.0	.0	.0	.0	AmLac++ MgEDTA-
1286	1	.0	.0	.0	.0	AmLac++ UmuAn#1-
1287	1	-3219	.0	.0	.0	AmOX- Cl-
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- NCO3-
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- B(OH)4-
1295	2	.0	.0	.0	.0	AmOX- B(OH)4-
1296	1	.0	.0	.0	.0	AmOX- B(OH)4-
1297	1	.0	.0	.0	.0	AmOX- Br-
1298	1	.0	.0	.0	.0	AmOX- Am(CO3)2-
1299	1	.0	.0	.0	.0	AmOX- Am(CO3)3--
1300	1	.0	.0	.0	.0	AmOX- ClO4-
1301	1	.0	.0	.0	.0	AmOX- NpO2(OH)2-
1302	1	.0	.0	.0	.0	AmOX- NpO2CO3-
1303	1	.0	.0	.0	.0	AmOX- NpO2(CO3)2--
1304	1	.0	.0	.0	.0	AmOX- NpO2(CO3)3---
1305	1	.0	.0	.0	.0	AmOX- H2PO4-
1306	1	.0	.0	.0	.0	AmOX- HPO4-
1307	1	.0	.0	.0	.0	AmOX- PO4--
1308	1	.0	.0	.0	.0	AmOX- Th(SO4)3-
1309	1	.0	.0	.0	.0	AmOX- Th(OH)3(CO3)-
1310	1	.0	.0	.0	.0	AmOX- Th(CO3)5---
1311	1	.0	.0	.0	.0	AmOX- HOx-
1312	1	.0	.0	.0	.0	AmOX- OX-
1313	1	.0	.0	.0	.0	AmOX- Ac-
1314	1	.0	.0	.0	.0	AmOX- Lac-
1315	1	.0	.0	.0	.0	AmOX- HCit-
1316	1	.0	.0	.0	.0	AmOX- HCit-
1317	1	.0	.0	.0	.0	AmOX- Cit-
1318	1	.0	.0	.0	.0	AmOX- H3EDTA-
1319	1	.0	.0	.0	.0	AmOX- H2EDTA-
1320	1	.0	.0	.0	.0	AmOX- HEDTA--
1321	1	.0	.0	.0	.0	AmOX- EDTA--
1322	1	.0	.0	.0	.0	AmOX- AmEDTA--
1323	1	.0	.0	.0	.0	AmOX- NpO2Cit-
1324	1	.0	.0	.0	.0	AmOX- NpO2EDTA---
1325	1	.0	.0	.0	.0	AmOX- NpO2OX-
1326	1	.0	.0	.0	.0	AmOX- U(OH)4(CO3)2--
1327	1	.0	.0	.0	.0	AmOX- U(CO3)5---
1328	1	.0	.0	.0	.0	AmOX- U(SO4)3-
1329	1	.0	.0	.0	.0	AmOX- Pu(CO3)2-
1330	1	.0	.0	.0	.0	AmOX- Pu(CO3)3--
1331	1	.0	.0	.0	.0	AmOX- PuEDTA-
1332	1	.0	.0	.0	.0	AmOX- CaCit-
1333	1	.0	.0	.0	.0	AmOX- CaEDTA-
1334	1	.0	.0	.0	.0	AmOX- UmuAn#2-
1335	1	.0	.0	.0	.0	AmOX- UmuAn#3-
1336	1	.0	.0	.0	.0	AmOX- UmuAn#4-
1337	1	.0	.0	.0	.0	AmOX- U(OH)2(CO3)2-
1338	1	.0	.0	.0	.0	AmOX- MgCit-
1339	1	.0	.0	.0	.0	AmOX- MgEDTA-
1340	1	.0	.0	.0	.0	AmOX- UmuAn#1-
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- NCO3-
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- B(OH)4-
1349	1	.0	.0	.0	.0	UCit- B(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

1361	1	.0	.0	.0	.0	UCit- Th(SO4)3-
1362	1	.0	.0	.0	.0	UCit- Th(OH)3(CO3)-
1363	1	.0	.0	.0	.0	UCit- Th(CO3)5===
1364	1	.0	.0	.0	.0	UCit- Hox-
1365	1	.0	.0	.0	.0	UCit- Ox-
1366	1	.0	.0	.0	.0	UCit- Ac-
1367	1	.0	.0	.0	.0	UCit- Lac-
1368	1	.0	.0	.0	.0	UCit- H2Cit-
1369	1	.0	.0	.0	.0	UCit- HCit-
1370	1	.0	.0	.0	.0	UCit- Cit-
1371	1	.0	.0	.0	.0	UCit- H3EDTA-
1372	1	.0	.0	.0	.0	UCit- H2EDTA-
1373	1	.0	.0	.0	.0	UCit- HEDTA-
1374	1	.0	.0	.0	.0	UCit- EDTA==
1375	1	.0	.0	.0	.0	UCit- AmEDTA-
1376	1	.0	.0	.0	.0	UCit- NpO2Cit-
1377	1	.0	.0	.0	.0	UCit- NpO2EDTA==
1378	1	.0	.0	.0	.0	UCit- NpO2Ox-
1379	1	.0	.0	.0	.0	UCit- U(OH)4(CO3)2==
1380	1	.0	.0	.0	.0	UCit- U(CO3)5===
1381	1	.0	.0	.0	.0	UCit- U(SO4)3-
1382	1	.0	.0	.0	.0	UCit- Pu(CO3)2-
1383	1	.0	.0	.0	.0	UCit- Pu(CO3)3--
1384	1	.0	.0	.0	.0	UCit- PuEDTA-
1385	1	.0	.0	.0	.0	UCit- CaCit-
1386	1	.0	.0	.0	.0	UCit- CaEDTA-
1387	1	.0	.0	.0	.0	UCit- UmuAn#2-
1388	1	.0	.0	.0	.0	UCit- UmuAn#3-
1389	1	.0	.0	.0	.0	UCit- UmuAn#4-
1390	1	.0	.0	.0	.0	UCit- U(OH)2(CO3)2-
1391	1	.0	.0	.0	.0	UCit- MgCit-
1392	1	.0	.0	.0	.0	UCit- MgEDTA-
1393	1	.0	.0	.0	.0	UCit- UmuAn#1-
1394						
1395	1	.2138	5.371	.0	.0	ULac+++ Cl-
1396	3	.0	.0	.0	.0	ULac+++ SO4-
1397	1	.0	.0	.0	.0	ULac+++ HSO4-
1398	1	.0	.0	.0	.0	ULac+++ OH-
1399	1	.0	.0	.0	.0	ULac+++ HCO3-
1400	1	.0	.0	.0	.0	ULac+++ CO3-
1401	1	.0	.0	.0	.0	ULac+++ B(OH)4-
1402	1	.0	.0	.0	.0	ULac+++ B3O3(OH)4-
1403	3	.0	.0	.0	.0	ULac+++ B4O5(OH)4-
1404	1	.0	.0	.0	.0	ULac+++ Br-
1405	1	.0	.0	.0	.0	ULac+++ Am(CO3)2-
1406	3	.0	.0	.0	.0	ULac+++ Am(CO3)3--
1407	1	.0	.0	.0	.0	ULac+++ ClO4-
1408	1	.0	.0	.0	.0	ULac+++ NpO2(OH)2-
1409	1	.0	.0	.0	.0	ULac+++ NpO2CO3-
1410	3	.0	.0	.0	.0	ULac+++ NpO2(CO3)2=-
1411	3	.0	.0	.0	.0	ULac+++ NpO2(CO3)3=-
1412	3	.0	.0	.0	.0	ULac+++ H2PO4-
1413	3	.0	.0	.0	.0	ULac+++ HPO4-
1414	3	.0	.0	.0	.0	ULac+++ PO4--
1415	3	.0	.0	.0	.0	ULac+++ Th(SO4)3-
1416	1	.0	.0	.0	.0	ULac+++ Th(OH)3(CO3)-
1417	3	.0	.0	.0	.0	ULac+++ Th(CO3)5===
1418	1	.0	.0	.0	.0	ULac+++ Hox-
1419	1	.0	.0	.0	.0	ULac+++ Ox-
1420	1	.0	.0	.0	.0	ULac+++ Ac-
1421	1	.0	.0	.0	.0	ULac+++ Lac-
1422	1	.0	.0	.0	.0	ULac+++ H2Cit-
1423	3	.0	.0	.0	.0	ULac+++ HCit-
1424	3	.0	.0	.0	.0	ULac+++ Cit-
1425	3	.0	.0	.0	.0	ULac+++ H3EDTA-
1426	3	.0	.0	.0	.0	ULac+++ H2EDTA-
1427	3	.0	.0	.0	.0	ULac+++ HEDTA-
1428	3	.0	.0	.0	.0	ULac+++ EDTA==
1429	3	.0	.0	.0	.0	ULac+++ AmEDTA-
1430	3	.0	.0	.0	.0	ULac+++ NpO2Cit-
1431	3	.0	.0	.0	.0	ULac+++ NpO2EDTA==
1432	3	.0	.0	.0	.0	ULac+++ NpO2Ox-
1433	3	.0	.0	.0	.0	ULac+++ U(OH)4(CO3)2==
1434	3	.0	.0	.0	.0	ULac+++ U(CO3)5===
1435	3	.0	.0	.0	.0	ULac+++ U(SO4)3-
1436	1	.0	.0	.0	.0	ULac+++ Pu(CO3)2-
1437	3	.0	.0	.0	.0	ULac+++ Pu(CO3)3--
1438	1	.0	.0	.0	.0	ULac+++ PuEDTA-
1439	1	.0	.0	.0	.0	ULac+++ CaCit-
1440	3	.0	.0	.0	.0	ULac+++ CaEDTA-
1441	3	.0	.0	.0	.0	ULac+++ UmuAn#2-
1442	1	.0	.0	.0	.0	ULac+++ UmuAn#3-
1443	3	.0	.0	.0	.0	ULac+++ UmuAn#4-
1444	3	.0	.0	.0	.0	ULac+++ U(OH)2(CO3)2-
1445	1	.0	.0	.0	.0	ULac+++ MgCit-
1446	3	.0	.0	.0	.0	ULac+++ MgEDTA-
1447	1	.0	.0	.0	.0	ULac+++ UmuAn#1-
1448						
1449	1	-.2061	-.525	.0	.0	UOx+++ Cl-
1450	2	.0	.0	.0	.0	UOx+++ SO4-
1451	1	.0	.0	.0	.0	UOx+++ HSO4-
1452	1	.0	.0	.0	.0	UOx+++ OH-
1453	1	.0	.0	.0	.0	UOx+++ HCO3-
1454	2	.0	.0	.0	.0	UOx+++ CO3-
1455	1	.0	.0	.0	.0	UOx+++ B(OH)4-
1456	1	.0	.0	.0	.0	UOx+++ B3O3(OH)4-
1457	2	.0	.0	.0	.0	UOx+++ B4O5(OH)4-
1458	1	.0	.0	.0	.0	UOx+++ Br-
1459	1	.0	.0	.0	.0	UOx+++ Am(CO3)2-
1460	3	.0	.0	.0	.0	UOx+++ Am(CO3)3--
1461	1	.0	.0	.0	.0	UOx+++ ClO4-
1462	1	.0	.0	.0	.0	UOx+++ NpO2(OH)2-
1463	1	.0	.0	.0	.0	UOx+++ NpO2CO3-
1464	3	.0	.0	.0	.0	UOx+++ NpO2(CO3)2=-
1465	3	.0	.0	.0	.0	UOx+++ NpO2(CO3)3=-
1466	1	.0	.0	.0	.0	UOx+++ H2PO4-
1467	2	.0	.0	.0	.0	UOx+++ HPO4-
1468	3	.0	.0	.0	.0	UOx+++ PO4--
1469	2	.0	.0	.0	.0	UOx+++ Th(SO4)3-
1470	1	.0	.0	.0	.0	UOx+++ Th(OH)3(CO3)-
1471	3	.0	.0	.0	.0	UOx+++ Th(CO3)5===
1472	1	.0	.0	.0	.0	UOx+++ Hox-
1473	2	.0	.0	.0	.0	UOx+++ Ox-
1474	1	.0	.0	.0	.0	UOx+++ Ac-
1475	1	.0	.0	.0	.0	UOx+++ Lac-
1476	1	.0	.0	.0	.0	UOx+++ H2Cit-
1477	2	.0	.0	.0	.0	UOx+++ HCit-
1478	3	.0	.0	.0	.0	UOx+++ Cit-
1479	3	.0	.0	.0	.0	UOx+++ H3EDTA-
1480	3	.0	.0	.0	.0	UOx+++ H2EDTA-
1481	3	.0	.0	.0	.0	UOx+++ HEDTA-
1482	3	.0	.0	.0	.0	UOx+++ EDTA==
1483	3	.0	.0	.0	.0	UOx+++ AmEDTA-
1484	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++ UmuAn#2-	
1496	3	.0	.0	.0	.0	UOX++ UmuAn#3-	
1497	2	.0	.0	.0	.0	UOX++ UmuAn#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++ UmuAn#1-	
1502							
1503	1	1.239	4.934	.0	.0	ThAc+++ Cl-	RCM96
1504	1	.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	3	.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	2	.0	.0	.0	.0	ThAc+++ NpO2EDTA=-	
1540	1	.0	.0	.0	.0	ThAc+++ NpO2Ox-	
1541	1	.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+++ UmuAn#2-	
1550	1	.0	.0	.0	.0	ThAc+++ UmuAn#3-	
1551	3	.0	.0	.0	.0	ThAc+++ UmuAn#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+++ UmuAn#1-	
1556							
1557	1	-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+ UmuAn#2-	
1604	1	.0	.0	.0	.0	ThCit+ UmuAn#3-	
1605	1	.0	.0	.0	.0	ThCit+ UmuAn#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

1733	1	.0	.0	.0	.0
1734	1	.0	.0	.0	.0
1735	1	.0	.0	.0	.0
1736	1	.0	.0	.0	.0
1737	1	.0	.0	.0	.0
1738	1	.0	.0	.0	.0
1739	1	.0	.0	.0	.0
1740	1	.0	.0	.0	.0
1741	1	.0	.0	.0	.0
1742	1	.0	.0	.0	.0
1743	1	.0	.0	.0	.0
1744	1	.0	.0	.0	.0
1745	1	.0	.0	.0	.0
1746	1	.0	.0	.0	.0
1747	1	.0	.0	.0	.0
1748	1	.0	.0	.0	.0
1749	1	.0	.0	.0	.0
1750	1	.0	.0	.0	.0
1751	1	.0	.0	.0	.0
1752	1	.0	.0	.0	.0
1753	1	.0	.0	.0	.0
1754	1	.0	.0	.0	.0
1755	1	.0	.0	.0	.0
1756	1	.0	.0	.0	.0
1757	1	.0	.0	.0	.0
1758	1	.0	.0	.0	.0
1759	1	.0	.0	.0	.0
1760	1	.0	.0	.0	.0
1761	1	.0	.0	.0	.0
1762	1	.0	.0	.0	.0
1763	1	.0	.0	.0	.0
1764	1	.0	.0	.0	.0
1765	1	.0	.0	.0	.0
1766	1	.0	.0	.0	.0
1767	1	.0	.0	.0	.0
1768	1	.0	.0	.0	.0
1769	1	.0	.0	.0	.0
1770	1	.0	.0	.0	.0
1771	1	.0	.0	.0	.0
1772	1	.0	.0	.0	.0
1773	1	.0	.0	.0	.0
1774	1	.0	.0	.0	.0
1775	1	.0	.0	.0	.0
1776	1	.0	.0	.0	.0
1777	1	.0	.0	.0	.0
1778	1	.0	.0	.0	.0
1779	1	.0	.0	.0	.0
1780	1	.0	.0	.0	.0
1781	1	.0	.0	.0	.0
1782	1	.0	.0	.0	.0
1783	1	.0	.0	.0	.0
1784	1	.0	.0	.0	.0
1785	1	.0	.0	.0	.0
1786	1	.0	.0	.0	.0
1787	1	.0	.0	.0	.0
1788	1	.0	.0	.0	.0
1789	1	.0	.0	.0	.0
1790	1	.0	.0	.0	.0
1791	1	.0	.0	.0	.0
1792	1	.0	.0	.0	.0
1793	1	.0	.0	.0	.0
1794	1	.0	.0	.0	.0
1795	1	.0	.0	.0	.0
1796	1	.0	.0	.0	.0
1797	1	.0	.0	.0	.0
1798	1	.0	.0	.0	.0
1799	1	.0	.0	.0	.0
1800	1	.0	.0	.0	.0
1801	1	.0	.0	.0	.0
1802	1	.0	.0	.0	.0
1803	1	.0	.0	.0	.0
1804	1	.0	.0	.0	.0
1805	1	.0	.0	.0	.0
1806	1	.0	.0	.0	.0
1807	1	.0	.0	.0	.0
1808	1	.0	.0	.0	.0
1809	1	.0	.0	.0	.0
1810	1	.0	.0	.0	.0
1811	1	.0	.0	.0	.0
1812	1	.0	.0	.0	.0
1813	1	.0	.0	.0	.0
1814	1	.0	.0	.0	.0
1815	1	.0	.0	.0	.0
1816	1	.0	.0	.0	.0
1817	1	.0	.0	.0	.0
1818	1	.0	.0	.0	.0
1819	1	.0	.0	.0	.0
1820	1	.0	.0	.0	.0
1821	1	.0	.0	.0	.0
1822	1	.0	.0	.0	.0
1823	1	.0	.0	.0	.0
1824	1	.0	.0	.0	.0
1825	1	.0	.0	.0	.0
1826	1	.0	.0	.0	.0
1827	1	-0.6	3.0	.0	0.2
1828	2	.0	.0	.0	.0
1829	1	.0	.0	.0	.0
1830	1	.0	.0	.0	.0
1831	1	.0	.0	.0	.0
1832	2	.0	.0	.0	.0
1833	1	.0	.0	.0	.0
1834	1	.0	.0	.0	.0
1835	2	.0	.0	.0	.0
1836	1	.0	.0	.0	.0
1837	1	.0	.0	.0	.0
1838	1	.0	.0	.0	.0
1839	1	.0	.0	.0	.0
1840	1	.0	.0	.0	.0
1841	1	.0	.0	.0	.0
1842	3	.0	.0	.0	.0
1843	3	.0	.0	.0	.0
1844	1	.0	.0	.0	.0
1845	2	.0	.0	.0	.0
1846	3	.0	.0	.0	.0
1847	2	.0	.0	.0	.0
1848	1	.0	.0	.0	.0
1849	3	.0	.0	.0	.0
1850	1	.0	.0	.0	.0
1851	2	.0	.0	.0	.0
1852	1	.0	.0	.0	.0
1853	1	.0	.0	.0	.0
1854	1	.0	.0	.0	.0
1855	2	.0	.0	.0	.0
1856	3	.0	.0	.0	.0

Am(OH)2+ NpO2CO3-
Am(OH)2+ NpO2 (CO3) 2--
Am(OH)2+ NpO2 (CO3) 3---
Am(OH)2+ H2PO4-
Am(OH)2+ HPO4-
Am(OH)2+ PO4--
Am(OH)2+ Th (SO4) 3=
Am(OH)2+ Th (OH) 3 (CO3) -
Am(OH)2+ Th (CO3) 5===
Am(OH)2+ HOx-
Am(OH)2+ Ox=
Am(OH)2+ Ac-
Am(OH)2+ Lac-
Am(OH)2+ H2Cit-
Am(OH)2+ HCit-
Am(OH)2+ Cit--
Am(OH)2+ H3EDTA-
Am(OH)2+ H2EDTA-
Am(OH)2+ HEDTA--
Am(OH)2+ EDTA--
Am(OH)2+ AmEDTA--
Am(OH)2+ NpO2Cit--
Am(OH)2+ NpO2EDTA--
Am(OH)2+ NpO2Ox-
Am(OH)2+ U (OH) 4 (CO3) 2==
Am(OH)2+ U (CO3) 5===
Am(OH)2+ U (SO4) 3=
Am(OH)2+ Pu (CO3) 2-
Am(OH)2+ Pu (CO3) 3--
Am(OH)2+ PuEDTA-
Am(OH)2+ CaCit-
Am(OH)2+ CaEDTA-
Am(OH)2+ UmuAn#2-
Am(OH)2+ UmuAn#3-
Am(OH)2+ UmuAn#4-
Am(OH)2+ U (OH) 2 (CO3) 2=
Am(OH)2+ MgCit-
Am(OH)2+ MgEDTA-
Am(OH)2+ UmuAn#1-
PuCO3+ Cl-
PuCO3+ SO4-
PuCO3+ HSO4-
PuCO3+ OH-
PuCO3+ HCO3-
PuCO3+ CO3=
PuCO3+ B (OH) 4-
PuCO3+ B1O3 (OH) 4-
PuCO3+ B4O5 (OH) 4=
PuCO3+ Br-
PuCO3+ Am (CO3) 2-
PuCO3+ Am (CO3) 3--
PuCO3+ ClO4-
PuCO3+ NpO2 (OH) 2-
PuCO3+ NpO2CO3-
PuCO3+ NpO2 (CO3) 2--
PuCO3+ NpO2 (CO3) 3---
PuCO3+ H2PO4-
PuCO3+ HPO4-
PuCO3+ PO4--
PuCO3+ Th (SO4) 3=
PuCO3+ Th (OH) 3 (CO3) -
PuCO3+ Th (CO3) 5===
PuCO3+ HOx-
PuCO3+ Ox=
PuCO3+ Ac-
PuCO3+ Lac-
PuCO3+ H2Cit-
PuCO3+ HCit-
PuCO3+ Cit--
PuCO3+ H3EDTA-
PuCO3+ H2EDTA-
PuCO3+ HEDTA--
PuCO3+ EDTA--
PuCO3+ AmEDTA--
PuCO3+ NpO2Cit-
PuCO3+ NpO2EDTA--
PuCO3+ NpO2Ox-
PuCO3+ U (OH) 4 (CO3) 2==
PuCO3+ U (CO3) 5===
PuCO3+ U (SO4) 3=
PuCO3+ Pu (CO3) 2-
PuCO3+ Pu (CO3) 3--
PuCO3+ PuEDTA-
PuCO3+ CaCit-
PuCO3+ CaEDTA-
PuCO3+ UmuAn#2-
PuCO3+ UmuAn#3-
PuCO3+ UmuAn#4-
PuCO3+ U (OH) 2 (CO3) 2=
PuCO3+ MgCit-
PuCO3+ MgEDTA-
PuCO3+ UmuAn#1-
PuOH++ Cl- analogy w/Am(III)
PuOH++ SO4-
PuOH++ HSO4-
PuOH++ OH-
PuOH++ HCO3-
PuOH++ CO3=
PuOH++ B (OH) 4-
PuOH++ B1O3 (OH) 4-
PuOH++ B4O5 (OH) 4=
PuOH++ Br-
PuOH++ Am (CO3) 2-
PuOH++ Am (CO3) 3--
PuOH++ ClO4-
PuOH++ NpO2 (OH) 2-
PuOH++ NpO2CO3-
PuOH++ NpO2 (CO3) 2--
PuOH++ NpO2 (CO3) 3---
PuOH++ H2PO4-
PuOH++ HPO4-
PuOH++ PO4--
PuOH++ Th (SO4) 3=
PuOH++ Th (OH) 3 (CO3) -
PuOH++ Th (CO3) 5===
PuOH++ HOx-
PuOH++ Ox=
PuOH++ Ac-
PuOH++ Lac-
PuOH++ H2Cit-
PuOH++ HCit-
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	1	.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++ UmuAn#2-
1874	1	.0	.0	.0	.0	PuOH++ UmuAn#3-
1875	1	.0	.0	.0	.0	PuOH++ UmuAn#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++ UmuAn#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+ B(O3(OH)4-
1889	1	.0	.0	.0	.0	Pu(OH)2+ B(O5(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+ NOx-
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+ HCl-
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+ UmuAn#2-
1928	1	.0	.0	.0	.0	Pu(OH)2+ UmuAn#3-
1929	1	.0	.0	.0	.0	Pu(OH)2+ UmuAn#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+ UmuAn#1-
1934						
1935	1	.227	2.154	.0	-.102	PuAc+ Cl- RCH96
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+ B(O3(OH)4-
1943	2	.0	.0	.0	.0	PuAc+ B(O5(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	1	.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+ NOx-
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	3	.0	.0	.0	.0	PuAc+ HCl-
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	3	.0	.0	.0	.0	PuAc+ U(SO4)3-
1976	1	.0	.0	.0	.0	PuAc+ Pu(CO3)2-
1977	3	.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	1	.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-	RCM96
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+ B(OH)3(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+ HOK-	
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+ HCit-	
2017	1	.0	.0	.0	.0	PuOx+ NCit-	
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-	RCM96
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)4-	
2050	1	.0	.0	.0	.0	PuLac++ B(OH)3(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++ HOK-	
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++ HCit-	
2071	1	.0	.0	.0	.0	PuLac++ NCit-	
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	1.696	.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+ B(OH)3(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+ ClO4-
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+ NOx-
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+ HCl-
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+ UmuAn#2-
2144	1	.0	.0	.0	.0	CaAc+ UmuAn#3-
2145	1	.0	.0	.0	.0	CaAc+ UmuAn#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+ UmuAn#1-
2150	1	.0	.0	.0	.0	CaLac+ Cl-
2151	1	.0	.0	.0	.0	CaLac+ SO4-
2152	1	.0	.0	.0	.0	CaLac+ HSO4-
2153	1	.0	.0	.0	.0	CaLac+ OH-
2154	1	.0	.0	.0	.0	CaLac+ HCO3-
2155	1	.0	.0	.0	.0	CaLac+ CO3-
2156	1	.0	.0	.0	.0	CaLac+ B (OH) 4-
2157	1	.0	.0	.0	.0	CaLac+ B3O3 (OH) 4-
2158	1	.0	.0	.0	.0	CaLac+ B4O5 (OH) 4*
2159	1	.0	.0	.0	.0	CaLac+ Br-
2160	1	.0	.0	.0	.0	CaLac+ Am (CO3) 2-
2161	1	.0	.0	.0	.0	CaLac+ Am (CO3) 3*-
2162	1	.0	.0	.0	.0	CaLac+ ClO4-
2163	1	.0	.0	.0	.0	CaLac+ NpO2 (OH) 2-
2164	1	.0	.0	.0	.0	CaLac+ NpO2CO3-
2165	1	.0	.0	.0	.0	CaLac+ NpO2 (CO3) 2*-
2166	1	.0	.0	.0	.0	CaLac+ NpO2 (CO3) 3***
2167	1	.0	.0	.0	.0	CaLac+ H2PO4-
2168	1	.0	.0	.0	.0	CaLac+ HPO4-
2169	1	.0	.0	.0	.0	CaLac+ PO4**
2170	1	.0	.0	.0	.0	CaLac+ Th (SO4) 3*
2171	1	.0	.0	.0	.0	CaLac+ Th (OH) 3 (CO3)-
2172	1	.0	.0	.0	.0	CaLac+ Th (CO3) 5***
2173	1	.0	.0	.0	.0	CaLac+ NOx-
2174	1	.0	.0	.0	.0	CaLac+ Ox-
2175	1	.0	.0	.0	.0	CaLac+ Ac-
2176	1	.0	.0	.0	.0	CaLac+ Lac-
2177	1	.0	.0	.0	.0	CaLac+ H2Cit-
2178	1	.0	.0	.0	.0	CaLac+ HCl-
2179	1	.0	.0	.0	.0	CaLac+ Cit**
2180	1	.0	.0	.0	.0	CaLac+ H3EDTA-
2181	1	.0	.0	.0	.0	CaLac+ H2EDTA-
2182	1	.0	.0	.0	.0	CaLac+ HEDTA**
2183	1	.0	.0	.0	.0	CaLac+ EDTA**
2184	1	.0	.0	.0	.0	CaLac+ AmEDTA**
2185	1	.0	.0	.0	.0	CaLac+ NpO2Cit-
2186	1	.0	.0	.0	.0	CaLac+ NpO2EDTA***
2187	1	.0	.0	.0	.0	CaLac+ NpO2Ox-
2188	1	.0	.0	.0	.0	CaLac+ U (OH) 4 (CO3) 2**
2189	1	.0	.0	.0	.0	CaLac+ U (CO3) 5***
2190	1	.0	.0	.0	.0	CaLac+ U (SO4) 3*
2191	1	.0	.0	.0	.0	CaLac+ Pu (CO3) 2-
2192	1	.0	.0	.0	.0	CaLac+ Pu (CO3) 3*-
2193	1	.0	.0	.0	.0	CaLac+ PuEDTA-
2194	1	.0	.0	.0	.0	CaLac+ CaCit-
2195	1	.0	.0	.0	.0	CaLac+ CaEDTA-
2196	1	.0	.0	.0	.0	CaLac+ UmuAn#2-
2197	1	.0	.0	.0	.0	CaLac+ UmuAn#3-
2198	1	.0	.0	.0	.0	CaLac+ UmuAn#4-
2199	1	.0	.0	.0	.0	CaLac+ U (OH) 2 (CO3) 2*
2200	1	.0	.0	.0	.0	CaLac+ MgCit-
2201	1	.0	.0	.0	.0	CaLac+ MgEDTA-
2202	1	.0	.0	.0	.0	CaLac+ UmuAn#1-
2203	1	.0	.0	.0	.0	
2204	1	.0	.0	.0	.0	
2205	1	.1696	.0	.0	.0	MgAc+ Cl- RCM96c
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+ ClO4-
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+ NOx-

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

2228	1	0	.0	.0	MgAc+ Ox-
2230	1	0	.0	.0	MgAc+ Ac-
2231	1	0	.0	.0	MgAc+ Lac-
2232	1	0	.0	.0	MgAc+ HCit-
2233	1	0	.0	.0	MgAc+ HCit-
2234	1	0	.0	.0	MgAc+ Cit-
2235	1	0	.0	.0	MgAc+ H3EDTA-
2236	1	0	.0	.0	MgAc+ H2EDTA-
2237	1	0	.0	.0	MgAc+ HEDTA-
2238	1	0	.0	.0	MgAc+ EDTA-
2239	1	0	.0	.0	MgAc+ AmEDTA-
2240	1	0	.0	.0	MgAc+ NpO2Cit-
2241	1	0	.0	.0	MgAc+ NpO2EDTA-
2242	1	0	.0	.0	MgAc+ NpO2Ox-
2243	1	0	.0	.0	MgAc+ U(OH)4(CO3)2-
2244	1	0	.0	.0	MgAc+ U(CO3)5---
2245	1	0	.0	.0	MgAc+ U(SO4)3-
2246	1	0	.0	.0	MgAc+ Pu(CO3)2-
2247	1	0	.0	.0	MgAc+ Pu(CO3)3-
2248	1	0	.0	.0	MgAc+ PuEDTA-
2249	1	0	.0	.0	MgAc+ CaCit-
2250	1	0	.0	.0	MgAc+ CaEDTA-
2251	1	0	.0	.0	MgAc+ UmuAn#2-
2252	1	0	.0	.0	MgAc+ UmuAn#3-
2253	1	0	.0	.0	MgAc+ UmuAn#4-
2254	1	0	.0	.0	MgAc+ U(OH)2(CO3)2-
2255	1	0	.0	.0	MgAc+ MgCit-
2256	1	0	.0	.0	MgAc+ MgEDTA-
2257	1	0	.0	.0	MgAc+ UmuAn#1-
2258					
2259	1	0	.0	.0	MgLac+ Cl-
2260	1	0	.0	.0	MgLac+ SO4-
2261	1	0	.0	.0	MgLac+ HSO4-
2262	1	0	.0	.0	MgLac+ OH-
2263	1	0	.0	.0	MgLac+ HCO3-
2264	1	0	.0	.0	MgLac+ CO3-
2265	1	0	.0	.0	MgLac+ B(OH)4-
2266	1	0	.0	.0	MgLac+ B3O3(OH)4-
2267	1	0	.0	.0	MgLac+ B4O5(OH)4-
2268	1	0	.0	.0	MgLac+ Br-
2269	1	0	.0	.0	MgLac+ Am(CO3)2-
2270	1	0	.0	.0	MgLac+ Am(CO3)3-
2271	1	0	.0	.0	MgLac+ ClO4-
2272	1	0	.0	.0	MgLac+ NpO2(OH)2-
2273	1	0	.0	.0	MgLac+ NpO2CO3-
2274	1	0	.0	.0	MgLac+ NpO2(CO3)2-
2275	1	0	.0	.0	MgLac+ NpO2(CO3)3---
2276	1	0	.0	.0	MgLac+ H2PO4-
2277	1	0	.0	.0	MgLac+ HPO4-
2278	1	0	.0	.0	MgLac+ PO4-
2279	1	0	.0	.0	MgLac+ Th(SO4)3-
2280	1	0	.0	.0	MgLac+ Th(OH)3(CO3)-
2281	1	0	.0	.0	MgLac+ Th(CO3)5---
2282	1	0	.0	.0	MgLac+ HOx-
2283	1	0	.0	.0	MgLac+ Ox-
2284	1	0	.0	.0	MgLac+ Ac-
2285	1	0	.0	.0	MgLac+ Lac-
2286	1	0	.0	.0	MgLac+ HCit-
2287	1	0	.0	.0	MgLac+ HCit-
2288	1	0	.0	.0	MgLac+ Cit-
2289	1	0	.0	.0	MgLac+ H3EDTA-
2290	1	0	.0	.0	MgLac+ H2EDTA-
2291	1	0	.0	.0	MgLac+ HEDTA-
2292	1	0	.0	.0	MgLac+ EDTA-
2293	1	0	.0	.0	MgLac+ AmEDTA-
2294	1	0	.0	.0	MgLac+ NpO2Cit-
2295	1	0	.0	.0	MgLac+ NpO2EDTA-
2296	1	0	.0	.0	MgLac+ NpO2Ox-
2297	1	0	.0	.0	MgLac+ U(OH)4(CO3)2-
2298	1	0	.0	.0	MgLac+ U(CO3)5---
2299	1	0	.0	.0	MgLac+ U(SO4)3-
2300	1	0	.0	.0	MgLac+ Pu(CO3)2-
2301	1	0	.0	.0	MgLac+ Pu(CO3)3-
2302	1	0	.0	.0	MgLac+ PuEDTA-
2303	1	0	.0	.0	MgLac+ CaCit-
2304	1	0	.0	.0	MgLac+ CaEDTA-
2305	1	0	.0	.0	MgLac+ UmuAn#2-
2306	1	0	.0	.0	MgLac+ UmuAn#3-
2307	1	0	.0	.0	MgLac+ UmuAn#4-
2308	1	0	.0	.0	MgLac+ U(OH)2(CO3)2-
2309	1	0	.0	.0	MgLac+ MgCit-
2310	1	0	.0	.0	MgLac+ MgEDTA-
2311	1	0	.0	.0	MgLac+ UmuAn#1-
2312					
2313	1	0	.0	.0	UnuCat#1+ Cl-
2314	1	0	.0	.0	UnuCat#1+ SO4-
2315	1	0	.0	.0	UnuCat#1+ HSO4-
2316	1	0	.0	.0	UnuCat#1+ OH-
2317	1	0	.0	.0	UnuCat#1+ HCO3-
2318	1	0	.0	.0	UnuCat#1+ CO3-
2319	1	0	.0	.0	UnuCat#1+ B(OH)4-
2320	1	0	.0	.0	UnuCat#1+ B3O3(OH)4-
2321	1	0	.0	.0	UnuCat#1+ B4O5(OH)4-
2322	1	0	.0	.0	UnuCat#1+ Br-
2323	1	0	.0	.0	UnuCat#1+ Am(CO3)2-
2324	1	0	.0	.0	UnuCat#1+ Am(CO3)3-
2325	1	0	.0	.0	UnuCat#1+ ClO4-
2326	1	0	.0	.0	UnuCat#1+ NpO2(OH)2-
2327	1	0	.0	.0	UnuCat#1+ NpO2CO3-
2328	1	0	.0	.0	UnuCat#1+ NpO2(CO3)2-
2329	1	0	.0	.0	UnuCat#1+ NpO2(CO3)3---
2330	1	0	.0	.0	UnuCat#1+ H2PO4-
2331	1	0	.0	.0	UnuCat#1+ HPO4-
2332	1	0	.0	.0	UnuCat#1+ PO4-
2333	1	0	.0	.0	UnuCat#1+ Th(SO4)3-
2334	1	0	.0	.0	UnuCat#1+ Th(OH)3(CO3)-
2335	1	0	.0	.0	UnuCat#1+ Th(CO3)5---
2336	1	0	.0	.0	UnuCat#1+ HOx-
2337	1	0	.0	.0	UnuCat#1+ Ox-
2338	1	0	.0	.0	UnuCat#1+ Ac-
2339	1	0	.0	.0	UnuCat#1+ Lac-
2340	1	0	.0	.0	UnuCat#1+ HCit-
2341	1	0	.0	.0	UnuCat#1+ HCit-
2342	1	0	.0	.0	UnuCat#1+ Cit-
2343	1	0	.0	.0	UnuCat#1+ H3EDTA-
2344	1	0	.0	.0	UnuCat#1+ H2EDTA-
2345	1	0	.0	.0	UnuCat#1+ HEDTA-
2346	1	0	.0	.0	UnuCat#1+ EDTA-
2347	1	0	.0	.0	UnuCat#1+ AmEDTA-
2348	1	0	.0	.0	UnuCat#1+ NpO2Cit-
2349	1	0	.0	.0	UnuCat#1+ NpO2EDTA-
2350	1	0	.0	.0	UnuCat#1+ NpO2Ox-
2351	1	0	.0	.0	UnuCat#1+ U(OH)4(CO3)2-
2352	1	0	.0	.0	UnuCat#1+ U(CO3)5---

INFORMATION ONLY

FMT, Version 2.3
User's Manual, Version 1.1

WPO # 43037
January 9, 1997
Page 279

Appendix W: Current Data Base, HMW_Am3Pu3Th4Np2_960823.CHEMDAT

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RF990N == Rai et al. 1996 Solubility of Th(IV) and U(IV) Hydrrous Oxides in Conc NaCl and MgCl2 Solutions
FR98MC96 == Felmy,Rai,Sterner,Mason,Hess,Conradson "Thermo Models for Highly Charged Aq Species
Solubility of Th(IV) Hydrrous Oxide in Conc NaHCO3 and Na2O3 Solns"

*V References
NR94 == Novak and Roberts (1994) SAND94-0805C MRS/Kyoto
FR95 == Fanghanel et al. (1995) RCA 6983 pp.169-176 "Thermo of Np(V): IIP's for Hydrolysis and Carbonate Complexes"
M95 == Novak 1995 memo of 1 OCT 95
LBL95 == Novak memo analyzing Np(V)/K2CO3 Experiments, 17OCT95

Organic Ligand References
CPN950705 == Novak memo to EJNovak
RCM96 == RC Moore, 22Feb96 memorandum "Final Model Parameters for Deprotonation of..."
RCM96b == RC Moore, 14Mar96 memo "Revision 1. Final Model Parameters..."
RCM96c == RC Moore, 17Mar96 memo "Model Parameters for Magnesium Complexation..."
RCM96d == Novak, Borkowski, Chopin RCA (1996) "Thermo Modeling of Np(V)-Acetate...in Conc NaCl"
MDC96 == Novak 16Apr96 memo "Thermo Params fo the Solubility of <<oxalate solids>>"
CPN16APR96 = Novak 16Apr96 memo "Thermo Params fo the Solubility of <<oxalate solids>>"

General References
HMW84 == Harvie, Moller, Weare (1984) GCA 48 pp.723-751
PM86 == Felmy and Weare (1986) GCA 50 pp.2771-2783
P76 == Pitzer and Silvester (1976) J Soln Chem 584 pp.269-278
P91 == Pitzer (1991) CRC Handbook, Activity Coef in Electrolyte Solns
CPN95a == Novak (1995a) 18Jan95 Memo "Creation and Definition of the Database for FMT called "HMW_NP_AM.CHEMDAT..."
NFR95 == Neck et al. (1995) RCA 6981 pp. 39-47, "Thermo of Np(V) in Conc Salt Solns..."

Appendix X: Current Data Base, HMW_Am3Pu3Th4Np5_960823.RHOMIN

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Appendix Y: Review Forms

This Appendix contains the review forms for the FMT User's Manual.