WASTE ISOLATION PILOT PLANT
Sandia National Laboratories

Software Cover Sheet

Form Number: 461-A Effective: 11/28/95

Procedure: 19-1 Revision: 2 Page 1 of 2

1. Document Name: User's Manual
2. Document Version Number: 1.0 3. WPO Number: 28119
4. Software Name: FMT 5. Version ID: 2.0
6. Software Classification[1]: SNL-SW
7. Summary of Contents

Number of pages in body of document: 195 Number of attachments: 1

Number of pages in each attachment: 26 Number of rolls of microfilm: NA

Number of pages of microfiche: NA

Number and format of electronic media items: NA

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

SANDRA C. BABB	Sandra C. Babb	4/15/96
Code Sponsor's Name *(print)*	*Signature*	Date
OS Dan W. Scott ~~Dan W. S~~	Dan W Scott	4-18-96
Preparer's Name *(print)*	*Signature*	Date
Preparer's Name *(print)*	*Signature*	Date

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

YIFENG WANG	Yifeng WS	4/15/96
Reviewer's Name *(print)*	*Signature*	Date
Kent G. Budge	Kent G Budge	15 Apr 1996
Reviewer's Name *(print)*	*Signature*	Date
Scott J Free	Scott J Free	4/15/96
Reviewer's Name *(print)*	*Signature*	Date

SWCF File Code: 1.4.01.6.1
WBS#

Software Cover Sheet

Form Number: 461-A
Effective: 11/28/95

10. Department Manager's Approval:

JOHN T. HOLMES	John T. Holmes	4/18/96
Department Manager's Name *(print)*	*Signature*	Date

11. SCM Coordinator's Signature:

Mario Chavez	Mario Chavez	5/3/96
SCM Coordinator's Name *(print)*	*Signature*	Date

(1) Choose from classifications in Appendix A.

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

WPO# 28119 Keywords: FMT, Chemical Equilbrium : Mass Balance : Free Energy Minimization

SWCF File Code SWCF- A : 1.4.01.6.1 : UM QA SET

A or C WBS #(s) Alpha Code(s)

WIPP PA

User's Manual

for

FMT, Version 2.0

Document Version 1.00

WPO # 28119

November 17, 1995

Table of Contents

List of Figures

List of Tables

1.0 INTRODUCTION

The program FMT (Fracture-Matrix Transport) solves chemical equilibrium problems using the Pitzer activity coefficient formalism (Pitzer, 1991). Although, as the name implies, this code was originally intended for transport calculations, this feature is not supported in this release of FMT (Version 2.0).

FMT is used to compute the concentrations, expressed in terms of molality (moles of solute per kilogram of solvent), of chemical species using a thermodynamic model for concentrated electrolyte systems (brines). FMT is used to simulate the solubility behavior of radionuclides in brines found in the Castile, Rustler, and Salado Formations near the WIPP site. FMT is based on the Harvie-Møller-Weare (HMW) data base (Harvie et al., 1984; Felmy and Weare, 1986) enhanced with radioactive elements such as americium(III) and neptunium(V). The purpose of the calculation is to find the detailed distribution of chemical species when the solution is at equilibrium.

FMT solves both single and multiple equilibrium problems:

- The single equilibrium problem (also known as the flash problem) uses the "batch" mode of FMT. In this mode, the user specifies the total element abundances and FMT calculates the equilibrium concentrations of dissolved components and solids.

- For multiple equilibrium problems a "titration" mode is available, in which FMT mechanizes repetitive flash calculations required to compute the composition of a solution results from titrating one solution with another solution or a solution containing minerals. For titration problems, the user specifies the compositions of both solutions and the volumes of the titrant solution to be added.

For the 1996 WIPP PA calculation, FMT will be used to generate tables of solubilities for generalized actinide (referred to here as "An") oxidation states An(III), An(IV), An(V), and An(VI). These tables will be converted into equations of surfaces that will be used by the WIPP PA codes PANEL and NUTS to calculate actinide solubility values as a function of CO_2 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 1996 WIPP Performance Assessment calculations. As such, it describes the code's purpose and function, the user's interaction with the code, and the equations and numerical methods employed by the code. Examples of user-accessible input files, output files, and screen displays are appended to this manual for the user's convenience.

1.1 Software Identifier

Code Name: FMT
WIPP Prefix: FMT_
Version Number: 2.0 11/03/95
Platforms: FORTRAN 77 for OpenVMS AXP, versions 1.5 and 6.1, on DEC Alpha and Power Macintosh 7100

1.2 Points of Contact

1.2.1 Code Sponsor

Sandra C. Babb
Sandia National Laboratories
Albuquerque, NM 87185-0661
Voice: (505) 844-7396 or (505) 848-0126
Fax: (505) 844-2018 or (505) 848-0881

1.2.2 Code Consultant

Craig F. Novak
Sandia National Laboratories
Albuquerque, NM 87185-1320
Voice: (505) 848-0619
Fax: (505) 848-0622

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) database enhanced 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: The element enhancements FMT supports include Americium (III) and Neptunium (V).

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

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

R.7: The "titrate" mode shall support linear increments, i.e., adding the same 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.

R.9: The parameters in the actinide series used in the FMT database are calculated by NONLIN or other equivalent means.

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
- 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 differential equations
- linear algebra (through senior undergraduate level)
- numerical methods (graduate or senior level undergraduate level).

4.0 DESCRIPTION OF THE MODELS AND METHODS

4.1 Mathematical Model and Numerical Methods

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

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

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

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

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

where

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

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

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

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

where

m = iteration index,

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

N' = number of species excluding inert species,

μ_i = chemical potential of species i, and

R = maximum number of linearly independent chemical equations.

The mole numbers are adjusted by means of

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

where n_i = the number of moles of species i.

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

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

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

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

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

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

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

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

where

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

T = absolute temperature (K)

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

n_k = number of moles of species k, and

n_t = total number of moles.

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

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

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

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

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

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

The 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 development of this model with a consistent data base as described by Harvie et al. (1984) and Felmy and Weare (1986) as the basis for modeling chemical nonidealities. These references provide extensive detail about this Pitzer activity coefficient formalism used in FMT. A brief discussion of the Pitzer activity coefficient model follows in Section 4.2.

4.2 The Pitzer Activity Coefficient Formalism

The Pitzer activity coefficient formalism is a set of mathematical equations for calculating activity coefficients for aqueous species, and is valid from dilute systems through the concentrated brines observed at the WIPP Site. The theoretical and historical development of this formalism can be traced though Pitzer (1991), particularly Chapter 3, 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:

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

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

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

and, for the solvent, by

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

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 neutrals), 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:

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

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.)

---

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

$$(\phi-1)=\frac{2}{\left(\sum_i m_i\right)}\left\{\frac{A^\phi I^{3/2}}{1+bI^{1/2}}+\sum_c\sum_a m_c m_a\left(B^\phi_{ca}+ZC_{ca}\right)+\sum_{c<c'}\sum m_c m_{c'}\left(\Phi^\phi_{cc'}+\sum_a m_a\psi_{cc'a}\right)\right.$$
$$+\sum_{a<a'}\sum m_a m_{a'}\left(\Phi^\phi_{aa'}+\sum_c m_c\psi_{aa'c}\right)+\sum_n\sum_c m_n m_c\lambda_{nc} \qquad \text{(A.2a)}$$
$$\left.+\sum_n\sum_a m_n m_a\lambda_{na}+\sum_n\sum_c\sum_a m_n m_c m_a\zeta_{nca}\right\}$$

$$\ln\gamma_M=z_M^2F+\sum_a m_a\left(2B_{Ma}+ZC_{Ma}\right)+\sum_c m_c\left(2\Phi_{Mc}+\sum_a m_a\psi_{Mca}\right)$$
$$+\sum_{a<a'}\sum m_a m_{a'}\psi_{aa'M}+|z_M|\sum_c\sum_a m_c m_a C_{ca}+\sum_n m_n\left(2\lambda_{nM}\right)+\sum_n\sum_a m_n m_a\zeta_{naM} \qquad \text{(A.2b)}$$

$$\ln\gamma_X=z_M^2F+\sum_c m_c\left(2B_{Xc}+ZC_{Xc}\right)+\sum_a m_a\left(2\Phi_{Xa}+\sum_c m_c\psi_{Xca}\right)$$
$$+\sum_{c<c'}\sum m_c m_{c'}\psi_{cc'X}+|z_X|\sum_c\sum_a m_c m_a C_{ca}+\sum_n m_n\left(2\lambda_{nX}\right)+\sum_n\sum_c m_n m_c\zeta_{ncX} \qquad \text{(A.2c)}$$

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

$$F=-A^\phi\left(\frac{I^{1/2}}{1+bI^{1/2}}+\frac{2}{b}\ln\left(1+bI^{1/2}\right)\right)+\sum_c\sum_a m_c m_a B'_{ca}$$
$$+\sum_{c<c'}\sum m_c m_{c'}\Phi'_{cc'}+\sum_{a<a'}\sum m_a m_{a'}\Phi'_{aa'} \qquad \text{(A.2e)}$$

$$C_{MX}=\frac{C^\phi_{MX}}{2|Z_M Z_X|^{1/2}} \qquad \text{(2b)}$$

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

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

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

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

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

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

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

The functions g and g' are defined by

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

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

with $x = \alpha_1\sqrt{I}$ or $= \alpha_2\sqrt{I}$. When either cation M or anion X is univalent, $\alpha_1 = 2.0$ and $\alpha_2 = 12$. For 2 - 2 pairs, $\alpha_1 = 1.4$ and $\alpha_2 = 12$. For all electrolyes, $b = 1.2$. For 2 - 3 and higher pairs, $\alpha_1 = 1.4$ and $\alpha_2 = 50$. The dimensions of α_1 and α_2 are $kg^{1/2}mole^{-1/2}$. The virial coefficients, Φ, which depend upon ionic strength, are given the following form:

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

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

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

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

The activity coefficient parameters, λ_{ni} and ζ_{nij}, representing the interactions between ions and neutral species, 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, Appendices I and J).

4.3 Inclusion of Pitzer Activity Coefficients

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

The following is an expression for the chemical potential:

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

and

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

or

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

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

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

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

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

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

where μ_i^* is now a function of T and P through the unknown equilibirum 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 $\vec{\gamma}$ 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

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

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

4.4 Charge Neutrality

Charge neutrality is maintained within FMT in order to best 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. 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 such as "PosIon+" and "NegIon-" made up of the pseudoelements PosIon:EL and NegIon:El and the appropriate charges can be used to do so. For example, entering a concentration of PosIon+ at 0.1m will cause the solution to have a net negative charge of 0.1m due to the nonfictitious species.

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.

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 current FMT data base, HMW_NP_AM.CHEMDAT (described in Section 7.3), is limited to the elements H, O, Na, K, Mg, Ca, Cl, B, and Br, and the pseudoelements "SO4," "CO3," "Am(III)," "Np(V)," "ClO4," and "Charge." (Element names contained in quotes are not strictly chemical elements, and are therefore called "pseudoelements." Pseudoelements are treated in the FMT data base 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 data base documentation (Appendix I) gives the sources of parameters contained in the data base. 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 imposing 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. These fictitious solids should have standard chemical potentials that are calculated from the gas fugacities.

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

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

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

At equilibrium, this reaction is described by the relationship

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

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

Other particular items to note are listed below:

- Oxidation-reduction (redox) reactions are not supported by the HMW_NP_AM data base.

- The "Am(III)" and "Np(V)" models in HMW_NP_AM are preliminary and provisional, and may be changed in further versions of the data base associated with FMT as more information becomes available. An example of this additional information is complexation with dissolved organic ligands such as the organic-acid anions acetate, lactate, oxalate, and citrate. Updated versions of the CHEMDAT data base for use with FMT will be issued as they are developed.

- The radioactive elements thorium(IV), 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. However, it is possible that several sections of code, particularly for calculating activity coefficients, may not be accessed until thorium(IV) is incorporated into the data base.

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 titrate problems. In the INPUT file the user sets the problem parameters and specifies the solution composition by providing the *total element* abundances.

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

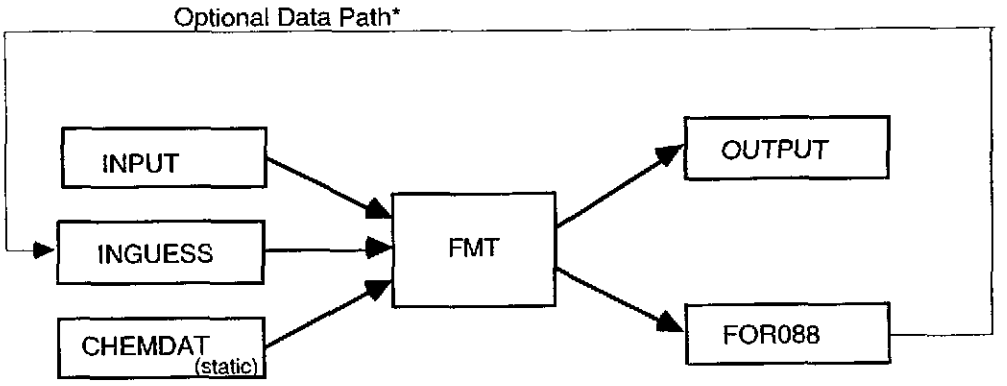
Optionally, the user could specify the same solution composition by setting the *species* abundances in the INGUESS file. The CHEMDAT file is a data base that contains species names, characteristics, and Pitzer parameters. RHOMIN, another data base file, contains mineral densities. FMT input files are discussed in detail in Section 7.0.

*****WARNING*****

The user should not and is not expected to change the CHEMDAT and RHOMIN files which are provided with the FMT code.

FMT generates a primary file OUTPUT and secondary file(s), depending on the problem. FOR088 is the secondary file for batch problems. TITRATE and MOLES are the secondary files 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 used as input for INGUESS. 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

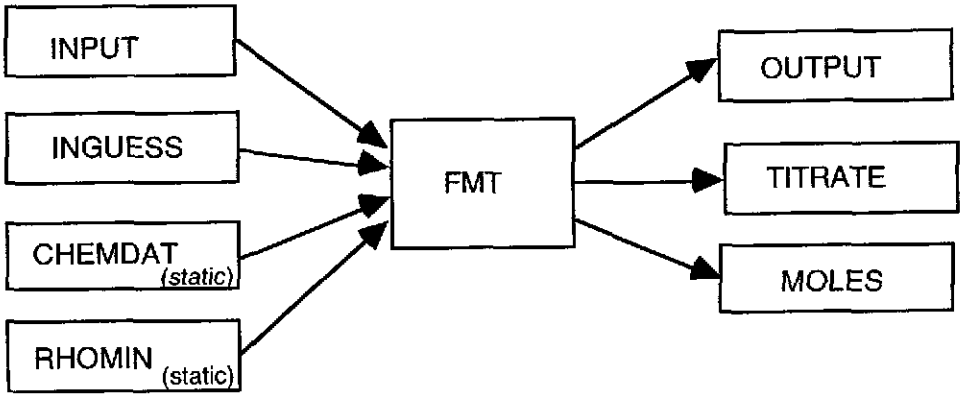


Figure 2. Input and Output Files for TITRATE

6.2 User-Supplied Input Files

Using a convenient editor, the user creates and modifies parameters in the INPUT and INGUESS files. After specifying a title for identifying the problem (usually naming the solution composition) and setting character flags in the INPUT file, the user quantifies the elemental amounts required for a specific solution. The user must specify the amounts in the same order as the elements are listed in the CHEMDAT file, starting with hydrogen.

The INGUESS file, if FMT is instructed to read it, provides molar amounts for each species in the CHEMDAT file. All amounts must be specified as total abundances, i.e., number of moles in the (unspecified) control volume. The user must state the moles for each species in the same order as

the species are listed in the CHEMDAT file, starting with H_2O. FMT converts these extrinsic quantities to molality using the mass of water that can form given the 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 DEC Environment

The user can use the command file FMT_FMTC.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_FMTC.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.

6.3.1.1 Fetching the Command File FMT_FMTC.COM from CMS

To retrieve the command file FMT_FMTC.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_fmtc.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_fmtc.com
```

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

6.3.1.2 Running FMT_FMTC.COM

To execute "@FMT_FMTC" 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_FMTC. To execute the command the user types in:

```
$@FMT_FMTC
```

The user will be prompted to supply a **substring** for the CHEMDAT and RHOMIN files and the input file's name. To retrieve a list of all CHEMDAT and RHOMIN files, the user can simply type in "FMT" since all database files are prefixed with the "FMT_HMW_" string. Any

substring of the database file name can be typed in if the user knows the valance states or the date of the files desired. The input file name must not contain the extensions (".IN" or ".INGUESS") and file names of IN and INGUESS must be the same.

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.

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

6.3.1.3 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_FMTC.COM generates the log file with the time and date stamp in the file's name. The log file records all the screen output, including explicit information on the build of the executable "FMT_FMT2P0" 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 after the run, the program FMT generated the files BATCH_DOC.OUT and BATCH_DOC.FOR088, CMS fetched the files FMT_HMW_NP_AM.CHEMDAT and FMT_HMW_NP_AM.RHOMIN, and FMT_FMTC.COM recorded the screen output from FMT in the file BATCH_DOC_JAN08_1519.LOG. A listing of the log file follows the directory listing.

```
$ dir

Directory U1:[SCBABB.FMT.CMS_TESTFILES]

BATCH_DOC.IN;1      BATCH_DOC.INGUESS;1 FMT_FMTC.COM;1

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

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW35_951213.CHEMDAT "K+ INTERACTIONS TO NP(V) SOLUBILITY DB"
FMT_HMW_35.CHEMDAT "Initial load"
FMT_HMW_35_951213.CHEMDAT "K+INTERACTIONS TO NP(V) SOLUBILITY W/O CMS HISTORY"
FMT_HMW_35_951213_F-1.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-10.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-11.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-12.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-13.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-14.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-2.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-3.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-4.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-5.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-6.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-7.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-8.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F-9.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F1.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_35_951213_F10.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
```

```
FMT_HMW_35_951213_F60.CHEMDAT "CO2 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK."
FMT_HMW_NP_AM.CHEMDAT "Initial load"
FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
Select CHEMDAT name from list above: FMT_HMW_NP_AM.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.CHEMDAT fetched

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_35.RHOMIN "Initial load"
FMT_HMW_NP_AM.RHOMIN "Initial load"
Select RHOMIN name from list above: FMT_HMW_NP_AM.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.RHOMIN fetched

                image name: "FMT_FMT2P0"
                image file identification: "PROD PA96"
                image file build identification: ""
                link date/time: 21-DEC-1995 11:36:28.86
                linker identification: "A11-14"

Entering Subroutine READDAT
reading chemical species data from CHEMDAT file
DG_BYPASS flag set to nDG_BYPASS
[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs                FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

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

ACTIVITY COEF. FLAG PITZACT
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

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

Echo of Mole Specifications:  nMOLES     nEXACT
ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH
  110.222364000000      Hydrogen
  55.1654821000000      Oxygen
 0.200000000000000      Sodium
 1.000000000000000E-002 Potassium
 1.000000000000000E-003 Magnesium
 1.000000000000000E-004 Calcium
 0.110000000000000      Chlorine
 1.000000000000000E-003 Sulfur
 1.000000000000000E-004 Carbon
 0.000000000000000E+000 PosIon
 0.000000000000000E+000 NegIon
 0.000000000000000E+000 Air
 1.000000000000000E-007 Boron
 0.000000000000000E+000 Bromine
 0.000000000000000E+000 TracerEl
 0.000000000000000E+000 Th(IV)
 0.000000000000000E+000 Am(III)
 0.000000000000000E+000 U(VI)
 0.000000000000000E+000 Np(V)
 0.000000000000000E+000 ClO4-(EL)
 0.000000000000000E+000 Phosphorus
 0.000000000000000E+000 Electron
 4.906053920000000E-017 Charge
.LT. (MINABU*1.d-6) moles NaBO2.NaCl.2H2O___Teepleite_(20_C); del&switch
.LT. (MINABU*1.d-6) moles NaB5O8.5H2O_____Sodium_Pentaborate; del&switch
.LT. (MINABU*1.d-6) moles NaOH(aq).....to.titrate.base.only; del&switch
.LT. (MINABU*1.d-6) moles HCl(aq).....to.titrate.acid.only; del&switch
.LT. (MINABU*1.d-6) moles K2B4O7.4H2O___K-Tetraborate_(30_C); del&reopt
.LT. (MINABU*1.d-6) moles B4O5(OH)4=              B4O5(OH)4=; del&reopt
.LT. (MINABU*1.d-6) moles K8H6(SO4)7_____________Misenite; del&reopt
.LT. (MINABU*1.d-6) moles K8H4(CO3)6.3H2O___K-Sequicarbonate; del&switch
.LT. (MINABU*1.d-6) moles B3O3(OH)4-             B3O3(OH)4-; del&switch
.LT. (MINABU*1.d-6) moles Ca4Cl2(OH)6.13H2O__CaOxychloride_A; del&switch

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

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

          2 Solubility Product Violations
Adding solid Mg(OH)2_____________________Brucite
pmH = -log[m(H+)]                =      12.7140
pH = -log[a(H+)]     =     12.8532
Total Diagonal Inversions           85
```

```
Total Stoichiometric Reoptimizations           10
SINGLE BATCH EQUILIBRATION COMPLETED
$ dir

Directory U1:[SCBABB.FMT.CMS_TESTFILES]

BATCH_DOC.FOR088;1  BATCH_DOC.IN;1       BATCH_DOC.INGUESS;1 BATCH_DOC.OUT;1
BATCH_DOC_JAN08_1519.LOG;1               FMT_FMTC.COM;1      FMT_HMW_NP_AM.CHEMDAT;1
FMT_HMW_NP_AM.RHOMIN;1

Total of 8 files.
$ type batch_doc_jan08_1519.log

                image name: "FMT_FMT2P0"
                image file identification: "PROD PA96"
                image file build identification: ""
                link date/time: 21-DEC-1995 11:36:28.86
                linker identification: "A11-14"

Entering Subroutine READDAT
reading chemical species data from CHEMDAT file
DG_BYPASS flag set to nDG_BYPASS
[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs                FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

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

ACTIVITY COEF. FLAG PITZACT
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

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

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

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

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

         2 Solubility Product Violations
Adding solid Mg(OH)2_____________________Brucite
pmH = -log[m(H+)]              =     12.7140
pH = -log[a(H+)]     =     12.8532
Total Diagonal Inversions          85
Total Stoichiometric Reoptimizations           10
SINGLE BATCH EQUILIBRATION COMPLETED
```

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, NP_NACL_BM.TITRATE, and NP_NACL_BM.MOLES.

```
$ dir

Directory U1:[SCBABB.FMT.CMS_TESTFILES]

FMT_FMTC.COM;1       FMT_HMW_NP_AM.CHEMDAT;1              FMT_HMW_NP_AM.RHOMIN;1
NP_NACL_BM.IN;5      NP_NACL_BM.INGUESS;2

Total of 5 files.
$ @fmt_fmtc
Enter chemdat file name to search on: np
Enter rhomin file name to search on: np
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_F60.CHEMDAT "Initial load"
Select CHEMDAT name from list above: FMT_HMW_NP_AM.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.CHEMDAT fetched

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.RHOMIN "Initial load"
Select RHOMIN name from list above: FMT_HMW_NP_AM.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.RHOMIN fetched

                image name: "FMT_FMT2P0"
                image file identification: "PROD PA96"
                image file build identification: ""
                link date/time: 21-DEC-1995 11:36:28.86
                linker identification: "A11-14"

Entering Subroutine READDAT
reading chemical species data from CHEMDAT file
DG_BYPASS flag set to nDG_BYPASS
Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

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

ACTIVITY COEF. FLAG PITZACT
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

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

Character Flags:  J.C. nMOLES     nEXACT
Character Flags:  I.C. nMOLES     nEXACT
TEMP is an unused local variable    180000.100000000

TITRATION option requires delta(x)=0.01 meters
  Defining delta(x) as such

DIFFUS  Parameter UNUSED= nDIFFUS
CONVEC  Parameter UNUSED= CONVEC
SSDIFF  Parameter UNUSED= nSSDIFF
RESTART Parameter Value Read = nRESTART
UNUSED Parameters nPUSHPULL nMULTINJ
UNUSED parameter FRAC FLO

TITRATION Problem:
 -) Assigning all delta(y) to 0.1 m
 -) Setting # of nodes in Y-direction to 3
 -) Setting NONREACTIVE Porosity to 0.0

Char Flags UNUSED UNUSED RHSFDIF    LHSFDIF
Char Flags UNUSED UNUSED nMOLES     nEXACT
```

```
TEMP is an unused local variable   9.9999999999999999E-021
Character Flags:  VPOROS FRFLASH VPOROS     FRFLASH

Specifying VARIABLE POROSITY for TITRATION Problem

Character Flags:  VAR_AQ_RHO VAR_AQ_RHO FRFLASH

Aqueous Density is a Function of Composition

Char Flag is UNUSED:  NO X DIFF nNO X DIFF
Char Flag is UNUSED:  UNIFORM UNIFORM              0

MINERAL DENSITIES, KG/M^3, IN FILE "RHOMIN"

pmH = -log[m(H+)]                  =     11.6199
pH = -log[a(H+)]     =     11.7497
pmH = -log[m(H+)]                  =      5.9141
pH = -log[a(H+)]     =      5.3205
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

pmH = -log[m(H+)]                  =      5.9141
pH = -log[a(H+)]     =      5.3205
pmH = -log[m(H+)]                  =      6.2386
pH = -log[a(H+)]     =      5.6451
pmH = -log[m(H+)]                  =      6.5870
pH = -log[a(H+)]     =      5.9936
pmH = -log[m(H+)]                  =      6.8286
pH = -log[a(H+)]     =      6.2353
pmH = -log[m(H+)]                  =      7.2930
pH = -log[a(H+)]     =      6.6996
pmH = -log[m(H+)]                  =      8.5359
pH = -log[a(H+)]     =      7.9427
pmH = -log[m(H+)]                  =      8.9250
pH = -log[a(H+)]     =      8.3317
pmH = -log[m(H+)]                  =      9.1587
pH = -log[a(H+)]     =      8.5655
pmH = -log[m(H+)]                  =      9.3098
pH = -log[a(H+)]     =      8.7166
pmH = -log[m(H+)]                  =      9.4653
pH = -log[a(H+)]     =      8.8722
pmH = -log[m(H+)]                  =      9.8154
pH = -log[a(H+)]     =      9.2225
pmH = -log[m(H+)]                  =     10.0620
pH = -log[a(H+)]     =      9.4695
pmH = -log[m(H+)]                  =     10.4406
pH = -log[a(H+)]     =      9.8493
pmH = -log[m(H+)]                  =     10.8825
pH = -log[a(H+)]     =     10.2955
pmH = -log[m(H+)]                  =     11.2341
pH = -log[a(H+)]     =     10.6594
End of AutoTitration Problem
$ dir

Directory U1:[SCBABB.FMT.CMS_TESTFILES]

FMT_FMTC.COM;1      FMT_HMW_NP_AM.CHEMDAT;1          FMT_HMW_NP_AM.RHOMIN;1
NP_NACL_BM.IN;5     NP_NACL_BM.INGUESS;2             NP_NACL_BM.MOLES;1
NP_NACL_BM.OUT;1    NP_NACL_BM.TITRATE;1             NP_NACL_BM_JAN08_1523.LOG;1

Total of 9 files.
```

6.3.2 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 and double clicking on a file name.

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

1. Select CHEMDAT File
2. Select RHOMIN File*
3. Select INPUT File
4. Select INGUESS File
5. Enter OUTPUT File Name
6. Enter FOR088 File Name

A titrate problem directs the user to:

1. Select CHEMDAT File
2. Select RHOMIN File
3. Select INPUT File
4. Select INGUESS File
5. Enter OUTPUT File Name
6. Enter TITRATE File Name
7. Enter MOLES File Name

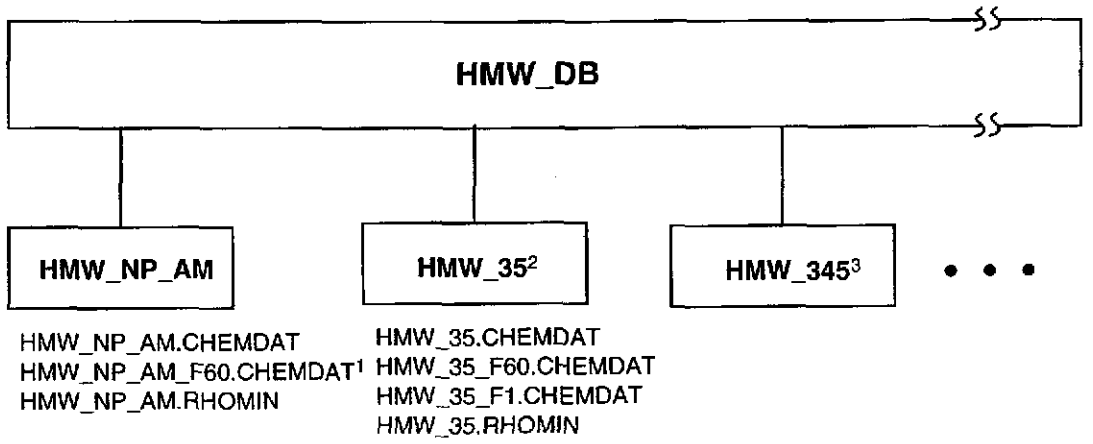
6.3.3 Organization of Files

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.

* 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.

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



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

Figure 3. Suggested data base organization.

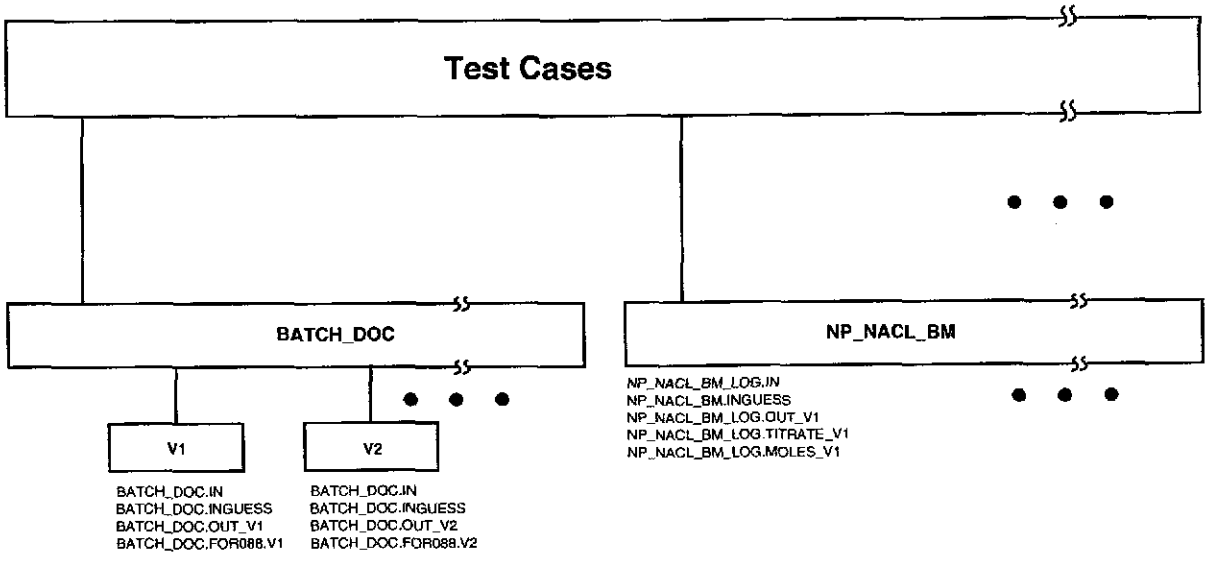


Figure 4. Suggested input/output file organization.

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 1 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.

Table 1. Batch Problem Screen Display Description (See Appendix A for sample listing.)

Line	Variable Name	Description
1	CHEMDAT_NAME	A partial string of a CHEMDAT filename to search on.
2	RHOMIN_NAME	A partial string of a RHOMIN filename to search on.
3	FILE_NAME	The full file name without the ".xxx" extension.
4-6		notation; setting pointers to FMT CMS library
8-11		list of CHEMDAT files with their comments in FMT CMS library that correspond to search string in line 1
12	CHEMDAT_NAME	user double clicks or cuts and pastes with a mouse or types in appropriate CHEMDAT filename
13-16		notation indicating that the CHEMDAT filename in line 12 has been copied to the user's current directory
18-20		list of RHOMIN files with their comments in FMT CMS library that correspond to search string in line 2
21	RHOMIN_NAME	user double clicks or cuts and pastes with a mouse or types in appropriate RHOMIN filename

22-25		notation indicating that the RHOMIN filename in line 21 has been copied to the user's current directory
27-31		linker and identity information on the FMT2P0 executable in CMS
33		*notation; FMT will begin reading problem description from* INPUT file (BATCH_DOC.IN, Appendix E) and chemical data from CHEMDAT file (HMW_NP_AM.CHEMDAT, Appendix I)
34		notation; FMT read 'CHEMFILE' from INPUT file (BATCH_DOC.IN, Appendix E)
35	DUMMY2	FMT read 'nDG_BYPASS' from CHEMDAT file (HMW_NP_AM.CHEMDAT, Appendix I)
36		notation; repeat of line 1 of INPUT file (BATCH_DOC.IN, Appendix E)
37-42	DBASE1, DBASE2, ACCURACY, MINABU,NAQ	repeat of lines 3-8 OUTPUT file for CHEMDAT (Appendix J)
44-45	DUMMY2	FMT read 'PITZACT' from CHEMDAT file (HMW_NP_AM.CHEMDAT, Appendix I) and notation (repeat of line 1273 from OUTPUT file for CHEMDAT [Appendix J])
46	ELNAMES (RPLWCHG)	repeat of line 1274 from OUTPUT file for CHEMDAT (Appendix J)
48		notation; FMT finished reading CHEMDAT file (HMW_NP_AM.CHEMDAT, Appendix I)
49	CDUM1,CDUM2	character strings read from INPUT file (BATCH_DOC.IN, Appendix E) to set batch mode
50		notation that FMT has a BATCH problem
51	DUMMY, DUMMY1	character strings read from INPUT file (BATCH_DOC.IN, Appendix E) to *not* read species amounts from INGUESS
52-76		*notation; listing of elemental abundances*
	ABUND(i), *ELNAMES(i)*	j^{th} mole amount from INPUT file (BATCH_DOC.IN, Appendix E) and i^{th} element name from CHEMDAT file (HMW_NP_AM.CHEMDAT, Appendix I)
77-86	NAMES(i)	species deleted from equilibrium algorithm because their total number of moles NMOLES(i) became negligible(<MINABU×1×10^{-6})

88-95		repeat of lines 17-24 in OUTPUT file for Batch (BATCH_DOC.OUT, Appendix M)
96-97		repeat of lines 163-164 in OUTPUT file for Batch (BATCH_DOC.OUT, Appendix M)
98-99		repeat of lines 180-181 in OUTPUT file for Batch (BATCH_DOC.OUT, Appendix M)
100		notation; normal exit from batch mode

6.4.2 Using FOR088 File as INGUESS File

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

Suppose the user ran a batch problem and generated the output files OUTPUT and FOR088. The FOR088 file contains the number of moles of each species calculated from the equilibrium run. 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 system.

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 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,...,N_s, is added to each beaker. The first volume addition is always zero, that is, $\Delta V_1 \equiv 0$. At each titration step the specified volume is

added to each of the N_s beakers containing 1 liter of Erlenmeyer solution, and each beaker is reequilibrated. This volume addition assumes that the density of the titrant is 1000 grams per liter.

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

FMT provides the user three different methods for specifying the titrant volume. Table 2 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 2. Titrate Options

Option	Description	Method
LINEAR	add the same constant titrant volume for each iteration increment	$\Delta V_i = DV(2) \times (i-1)$, $i=2,\ldots,N_S$, where DV(2) is read from the INPUT file
LOG10	add titrant volumes that increase exponentially from the user specified minimum to maximum volumes	$\Delta V_i = DV(2) \times e^{(i-2)R}$, $i=2,\ldots,N_S$, 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	$\Delta V_i = DV(i)$, $i=2,\ldots,N_S$, 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'

$\Delta V_i = 0.1 \times e^{(i-2)R}$ with R=(ln(10.0)-ln(0.1))/13.0,

i=2,…,15 for 'LOG10'

and user-specified increments for 'ASREAD'.

The final volume is

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

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

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

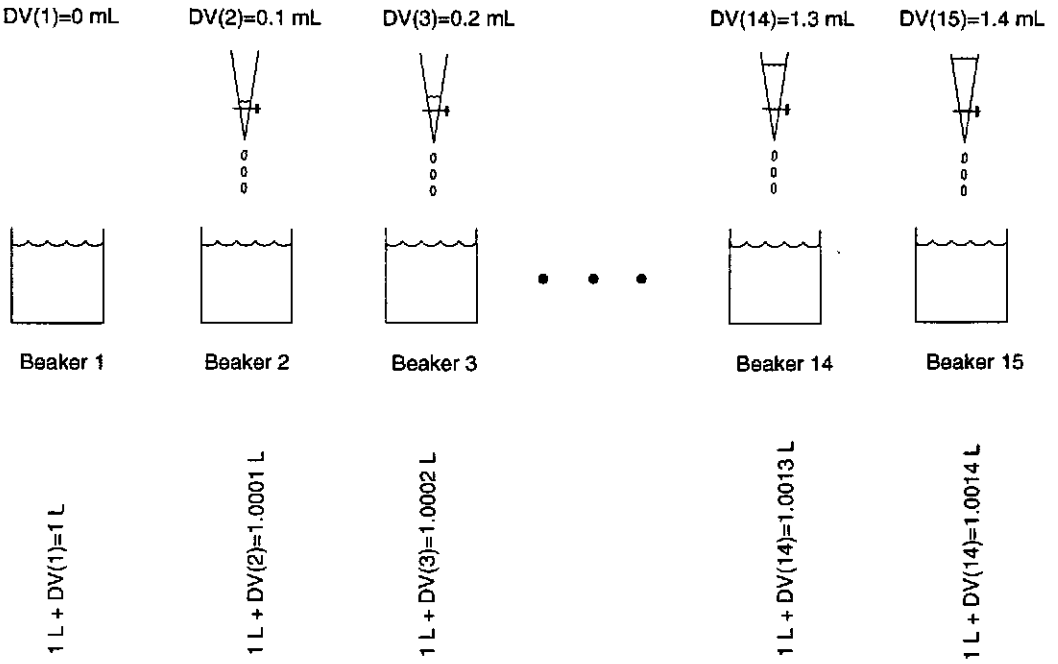


Figure 5. Titration problem using LINEAR option.

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 locate regions of slow and rapid pH changes
3. use the ASREAD option to show the minimum number of points of pH changes

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

where i=2, . . ., NSPACE.

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

6.5.2 Screen Display Descriptions

Table 3 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.

Table 3. 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
1-48		repeat of variable names and descriptions in Table 1 for Batch
49	CDUM1,CDUM2	character strings read from 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
50		notation that FMT has a TITRATION problem
52	CDUM1,CDUM2	character strings read from INPUT (Appendices F, G, or H) to *not* read species amounts from INGUESS for the injected or buret solution
53	CDUM1,CDUM2	character strings read from INPUT (Appendices F, G, or H) to *not* read species amounts from INGUESS for the initial or Erlenmeyer solution
54		unused number read from INPUT (Appendices F, G, or H) line 56
56-57		notation; repeated in OUTPUT file for CHEMDAT (Appendix J)
59-64		unused character strings read from INPUT (Appendices F, G, or H) lines 57-61,65
66-69		repeat of lines 17-20 in OUTPUT file for Titrate (Np_NaCl_BM_LOG.OUT [Appendix N], Np_NaCl_BM_LIN.OUT [Appendix O], or Np_NaCl_BM.OUT [Appendix P])

71-72		unused character strings read from INPUT (Appendices F, G, or H) line 68-69
74-75		unused variables read from INPUT (Appendices F, G, or H) line 94-95
77		notation; repeat of line 18 in OUTPUT file for Titrate (Appendices N, O, or P)
79		unused variables read from INPUT (Appendices F, G, or H) lines 95-96
81		notation; repeat of line 24 in OUTPUT file for Titrate (Appendices N, O, or P)
83-84		unused character string read from INPUT (Appendices F, G, or H) line 97-98
86		notation; repeat of line 27 in OUTPUT file for Titrate (Appendices N, O, or P)
88-89		pmH (negative base 10 logarithm of hydrogen ion molality) and pH (negative base 10 logarithm of hydrogen ion activity) of the titrant solution
90-91		*pmH and pH of the Erlenmeyer solution*
93	CDUM1,CDUM2	character strings read from INPUT (Appendices F, G, or H) to set titrate method
94-95	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
97-126		pmH and pH of *resulting solutions following titrant additions* DV(i), i=1, . . ., N_S to 1 liter of the Erlenmeyer solution, with no additions to the first beaker; see Figure 5.
127		*notation; normal exit from titrate mode*

6.5.3 Titrate Sample Problem: Solubility Calculation

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

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

Referring to Appendix P, 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 58 and 102, approximately 2 molal CO_3^{2-} on Line 103, with 1.61 molal Cl^- (Lines 62 and 104) to create a charge-neutral solution. The titrant was designed to have a very high carbonate concentration. The solution could not have been made much more concentrated in carbonate because it is nearly saturated with respect to $Na_2CO_3 \cdot 7H_2O(s)$ as indicated by the Saturation Index of –0.251 listed in the Descriptor column on Line 114. The flash calculation output for the Erlenmeyer solution shows 5.61 molal sodium and 5.61 molal chloride (Lines 198 and 197), in equilibrium with a large excess of $NaNpO_2CO_3(s)$ at a relatively high pmH of 5.91 on Line 222. This solution was designed to have a very low carbonate concentration, 3.09×10^{-8} molal (Line 204). A large excess of $NaNpO_2CO_3(s)$ was specified because we are investigating the solubility behavior of this solid as conditions vary, and the large excess allows the amount of solid to change with changing aqueous conditions while keeping the solid phase present.

Examining the TITRATE file, Appendix T, the listing for Np_NaCl_BM.TITRATE on Lines 26-41, shows that the Na^+ concentration remains constant at 5.61 molal, while the Cl^- concentration changes slightly from 5.61 to 5.51 molal. More importantly, the CO_3^{2-} concentration varies widely, from 3.09×10^{-8} to 4.84×10^{-2} molal (Lines 43-58), as was intended. The $NaNpO_2CO_3(s)$ concentrations confirm that this solid is present across this aqueous composition range (Lines 79-94), and all other solid phases are absent. The concentrations of the Np(V) species NpO_2^+, $NpO_2OH(aq)$, $NpO_2(OH)_2^-$, $NpO_2CO_3^-$, $NpO_2(CO_3)_2^{3-}$, and $NpO_2(CO_3)_3^{5-}$, given in Lines 62-77 are the desired information from this simulation; these are plotted in Figure 6, along with the total Np(V) in solution (the sum of the individual species concentrations) and experimental measurements of this system from Neck et al. (1994).

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

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

Figure 6 is comparable to Figure 7 from Novak and Roberts (1995), the main difference being the axis ranges. This figure shows that the hydrolysis species $NpO_2OH(aq)$ and $NpO_2(OH)_2^-$ are unimportant under these conditions, with concentrations always at least three orders of magnitude smaller than the total Np(V). This example shows the comparison between model calculations and experimental data, and also shows that the values calculated with FMT Version 1.0, used in

Novak and Roberts (1995), agree with values calculated with FMT Version 2.0, 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 T.

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

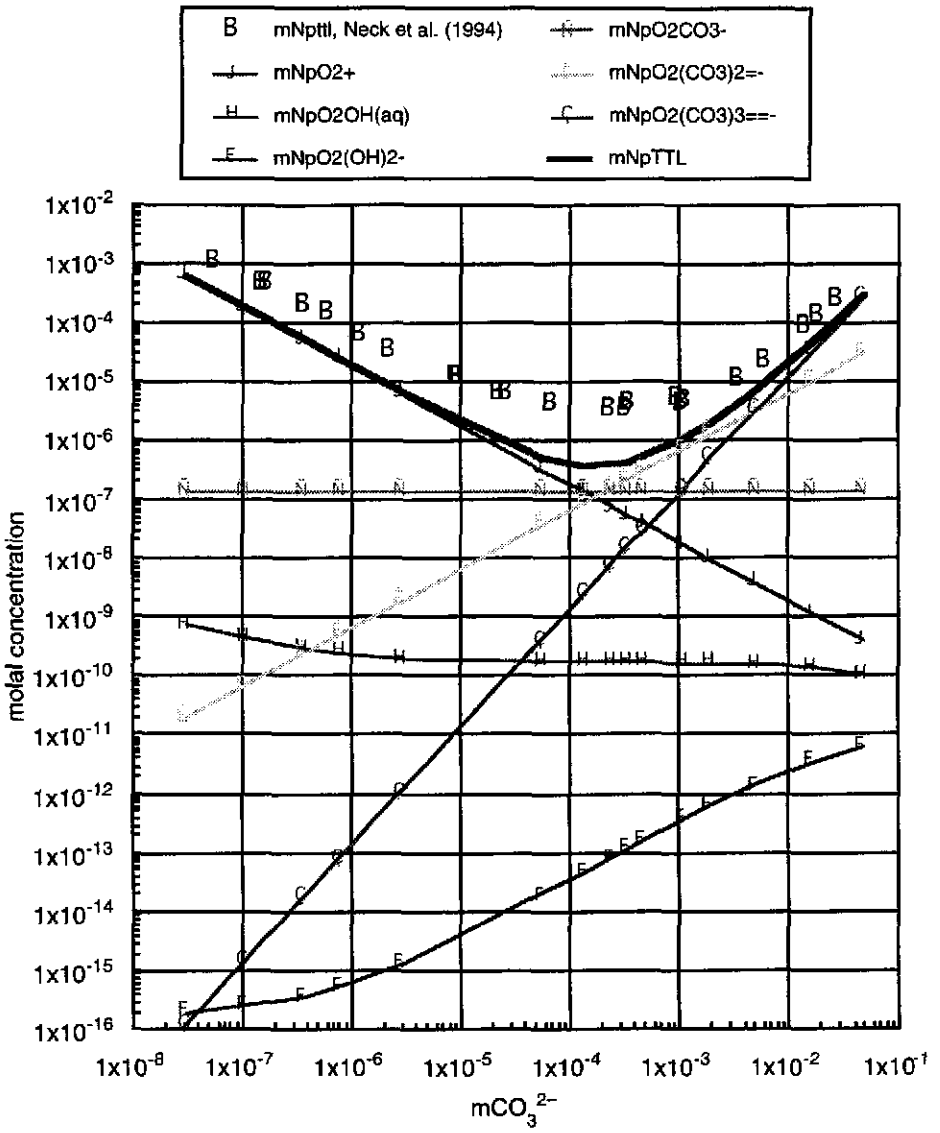


Figure 6. Calculated Total Np(V) and Np(V) Concentrations as a function of CO_3^{2-} concentration in 5.61 molal (5M) NaCl, and comparison with experimental measurements from Neck et al. (1994).

7.0 DESCRIPTION OF INPUT FILES

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

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

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

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

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

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

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

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

7.1 INPUT

7.1.1 Batch Problem

The batch INPUT (.IN) file is used to specify the molar abundances of the elements for the batch problem. The bulk of the lines in this file (Figure 7) specifies element abundances. The flags on Line 6 indicate if the INGUESS file should be read for species abundances. A line-by-line description of this file is provided below in Table 4, and a sample listing of BATCH_DOC.IN is provided in Appendix E.

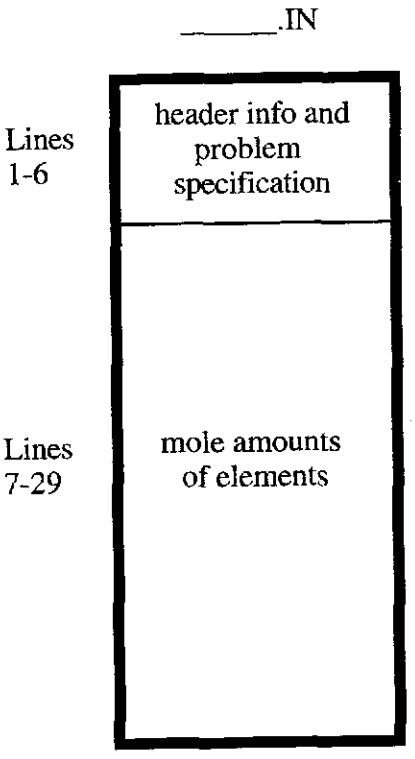


Figure 7. Batch INPUT file.

Table 4 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.

Table 4. 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		2 character strings used as flags for calculating the equilibrium state using either:
		'MOLES' 'EXACT'	species abundances read from INGUESS from which FMT calculates element abundances
		or	
		'nMOLES' 'nEXACT'	element abundances from INPUT (does not read INGUESS)
7-29	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

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

7.1.2 Titrate Problem

The titrate INPUT (.IN) file, a required input file for running a titrate calculation (Section 6.1), 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) specifies the molar abundances of the elements in the buret and Erlenmeyer ("beaker") solutions. Line 6 or Line 31 allows the user to set flags that force a read of the INGUESS file for species abundances. Line 100 in the file allows the user to specify that the titration method — adding equal volumes of the titrant successively (LINEAR), adding titrant volumes that increase exponentially (LOG10), or adding user-specified titrant volumes (ASREAD). A line-by-line description of this file is provided in Table 5, and sample listings are provided in Appendix F (LOG10 method), Appendix G (LINEAR method), and Appendix H (ASREAD).

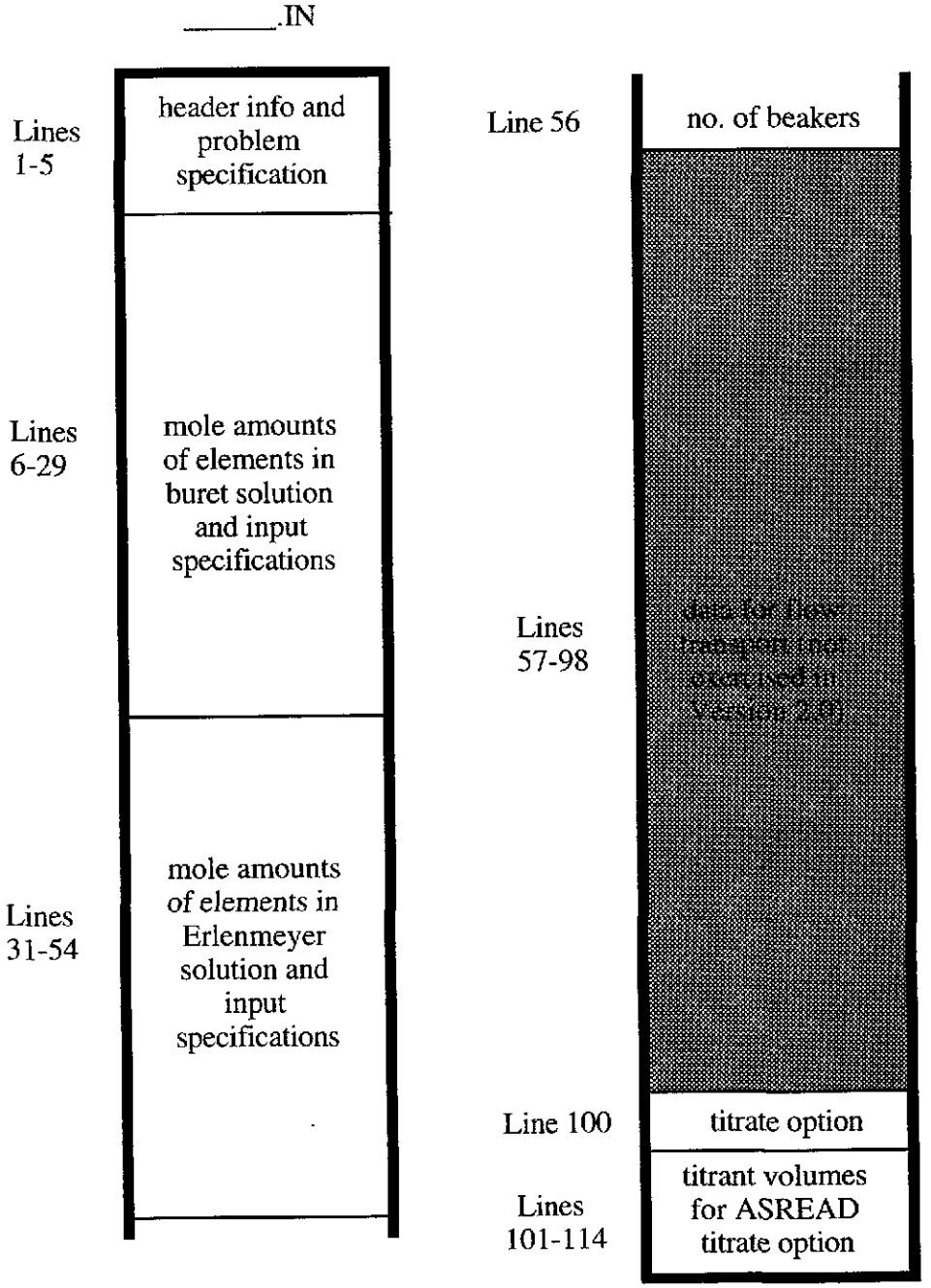


Figure 8. Titrate INPUT file.

The INPUT file parameters for a titrate problem are shown in Table 5. The "LINE" column in Table 5 refers to the lines listed in the Np_NaCl_BM_LOG.IN, Np_NaCl_BM_LIN.IN, and Np_NaCl_BM.IN files.

Table 5. INPUT File Parameters for Titrate (See Appendices F, G, and H for sample listings of Np_NaCl_BM_LOG.IN, Np_NaCl_BM_LIN.IN, and Np_NaCl_BM.IN, respectively.)

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

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

32-54	ELTOTAL (i,2)	nonnegative real number**	mole amount of i^{th} element in Erlenmeyer solution, one elemental amount per line
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 are 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.

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

	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.

In the input files referenced in the above table, lines 6-29 state the composition of the titrant or buret solution. Lines 31-54 define the composition of the titrated or Erlenmeyer solution. Line 56 states the number of beakers, N_S, for titration. Lines 57 through 98 are read but not used.

The INPUT file structure accommodates the three titration methods:

- Line 100 in the file Np_NaCl_BM_LOG.IN demonstrates using the 'LOG10' option with the initial and final volumes. FMT disregards any lines following line 100.
- Line 100 in the file Np_NaCl_BM_LIN.IN 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.
- Line 100 in the file Np_NaCl_BM.IN sets the 'ASREAD' option, and FMT disregards the initial and final volume numbers. In lines 100-114 of the Np_NaCl_BM.IN file, FMT reads the 14 user-specified volumes for the 'ASREAD' option.

7.2 INGUESS

The INGUESS file is an input file for both the batch and titrate options that allows the user to specify the species abundances, from which FMT calculates the element abundances. The user must set the appropriate flags 'MOLES' and 'EXACT' in the INPUT file (Section 7.1). (If the INGUESS file is not used, the element abundances provided in the INPUT file are used.)

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 Q), is provided below in Table 6.

Table 6. 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 (or FOR088) file, the total moles is followed by a species name and molality value. The order of the species listed follows that of the CHEMDAT file (Appendix I, Lines 14-140). HMW_NP_AM.CHEMDAT file has 115 species. FMT does not read the names or molality values from an INGUESS file, which were derived from a renamed FOR088 file.

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 5. '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 7. INGUESS File Parameters for Titrate Problem

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

7.3 Standard CHEMDAT Input File

FMT is capable of evaluating the HMW model as defined in the CHEMDAT file, which contains the thermodynamic parameters necessary to model the chemical behavior of actinide elements in brines. 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 term HMW_NP_AM.CHEMDAT as used throughout this document refers to version 95.01.31 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).

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.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.CHEMDAT, version date 95.01.31.

*****NOTE*****
HMW_NP_AM.CHEMDAT is not necessarily the CHEMDAT file that will be used to support the WIPP 1996 PA calculations. Additional species and elements will be added to the HMW_NP_AM.CHEMDAT that will be used to support the 1996 WIPP PA calculations.

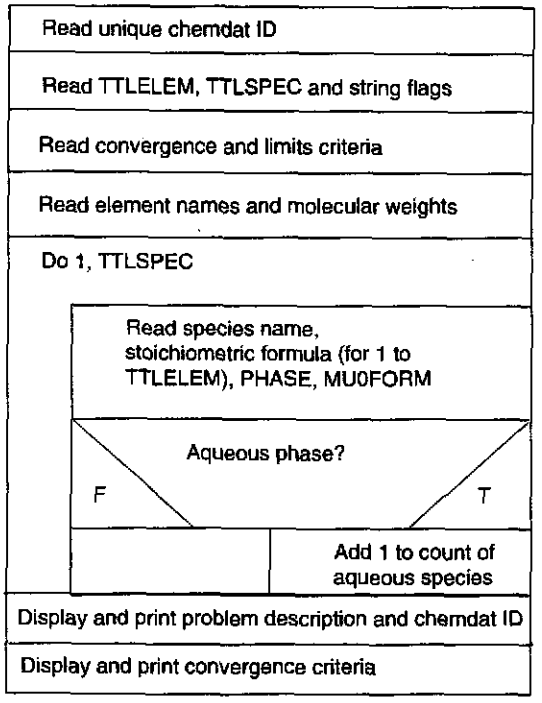
This data base contains the thermodynamic parameters necessary to model the chemical behavior of Np(V) and Am(III) in brines. Note that the extension of the Pitzer model to higher electrolyte types than in Harvie et al. (1984) and Felmy and Weare (1986) is necessary for Am(III); this is discussed in 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 the FMT subroutines READDAT and RDPITZR read from the CHEMDAT file. 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.



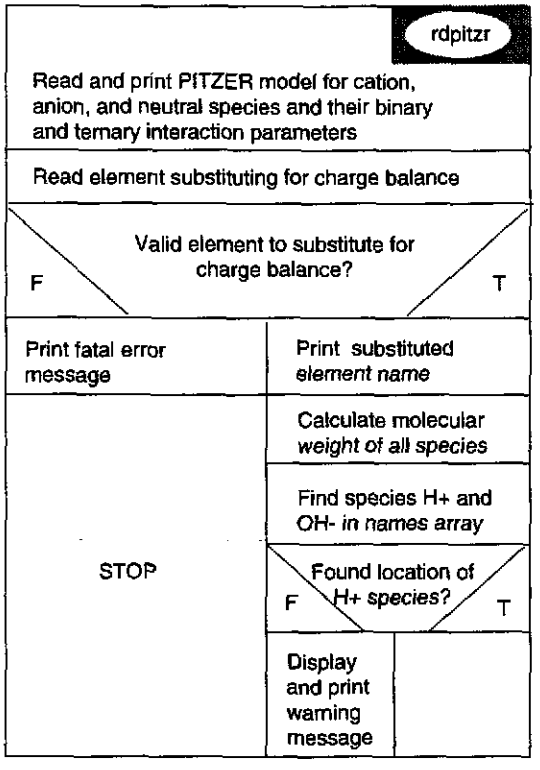


Figure 9. Nassi-Schneiderman (N-S) chart showing FMT control flow.

7.3.2 CHEMDAT Data Sources

The temperature range of the thermodynamic data is specified at 25 ° C with a few species at 20°C and 30°C.

The data for HMW_NP_AM.CHEMDAT can be grouped into three types: parameters for the brine (evaporite) electrolytes, parameters for Np(V) interactions with evaporite electrolytes, and parameters for Am(III) interactions with evaporite electrolytes. There is some overlap among these groups, but this categorization scheme will be used.

7.3.2.1 Brine Model

Parameters for brine electrolytes come primarily from Harvie et al. (1984) and Felmy and Weare (1986), called Harvie-Møller-Weare/Felmy-Weare, or HMW/FW or simply HMW for short. Harvie et al. (1984) presents a model for the Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O system, and Felmy and Weare (1986) extends this model to include boron species. Also included in this category are data from Pitzer (1991) for ion interactions with perchlorate, ClO_4^-. Perchlorate data are included in HMW_NP_AM.CHEMDAT not because perchlorate is important for the WIPP, but because much actinide chemistry was measured in the presence of perchlorate, and therefore parameters are needed to interpret these data. Parameters from Harvie et al. (1984) and Felmy and Weare (1986) were taken directly with no modification, and are not reproduced here. Parameters from Pitzer (1991) were scaled as necessary from the forms in which they were reported to the forms needed for use by FMT. These parameters are documented in Table 8.

7.3.2.2 Np(V) Model

Parameters for Np(V) interactions in NaCl, $NaClO_4$, and Na_2CO_3 media are taken from Novak and Roberts (1995). This model for Np(V) chemistry in brines is limited to predominantly NaCl, $NaClO_4$, or Na_2CO_3 media, and has not been shown to apply to other media. However, it can provide a first estimate of the solubility behavior of neptunium(V) in predominantly sodium chloride groundwaters containing carbonate, such as brines from the Castile and Rustler Formations in the vicinity of the WIPP Site. Parameters for Np(V) were taken directly from Novak and Roberts (1995) with no modification, as given in Tables 9 and 10. Since the publication of Novak and Roberts (1995), several alternative sets of parameters for Np(V) in concentrated electrolytes have been released in draft form. These will be included in future releases of the CHEMDAT data base for the purpose of WIPP PA calculations.

7.3.2.3 Am(III) Model

Parameters for Am(III) interactions with chloride, sulfate, phosphate, and carbonate anions, including interactions with several groundwater cations, are taken from Felmy et al. (1990), Felmy et al. (1989), Rai et al. (1992a, 1992b, 1994), and Rao et al. (1994). Although these parameters were developed for Am(III), Pu(III), or Nd(III), we have used the oxidation state analogy for f-elements (Novak and Dhooge, 1995) to apply these parameters to Am(III) as shown here. Although we call it the Am(III) model, this model should apply equally well to Pu(III) and Nd(III).

Felmy et al. (1990) provide the values of standard chemical potential for the americium species shown in Table 11, and the ion interaction parameters shown in Table 12. These parameters were developed from relatively dilute, i.e., less than 0.1 molal, solutions, so they do not necessarily apply to more concentrated solutions, as this discussion of Rao et al. (1994) below shows.

Rai et al. (1992b) use Nd(III) and Am(III) data from Felmy et al. (1990) and Rai et al. (1983) to develop the Nd(III) standard chemical potentials shown in Table 13. These values were converted to standard chemical potentials for the analogous Am(III) species for use within HMW_NP_AM.CHEMDAT as follows. One can write a general chemical reaction Nd^{3+} with a ligand Y^n, where n can be positive or negative, and the analogous reaction for Am^{3+}:

$$Nd^{3+} + yY^n \leftrightarrow NdY_y^{3+yn} \qquad \mu^o_{rxn1} = \mu^o_{NdY_y^{3+yn}} - \mu^o_{Nd^{3+}} - y\,\mu^o_{Y^n} \tag{15}$$

$$Am^{3+} + yY^n \leftrightarrow AmY_y^{3+yn} \qquad \mu^o_{rxn2} = \mu^o_{AmY_y^{3+yn}} - \mu^o_{Am^{3+}} - y\,\mu^o_{Y^n} \tag{16}$$

Because we are assuming identical chemical behavior for Am(III) and Nd(III), we must have $\mu^o_{rxn1} = \mu^o_{rxn2}$. Therefore, the standard chemical potential for the complex americium species is given by

$$\mu^o_{AmY_y^{3+yn}} = \mu^o_{NdY_y^{3+yn}} + \left[\mu^o_{Am^{3+}} - \mu^o_{Nd^{3+}}\right] \tag{17}$$

Analogous expressions hold for Pu(III). The dimensionless standard chemical potentials for the second and third americium hydrolysis species, calculated using the above equation, are given in Table 13.

Felmy et al. (1989) gives ion interaction parameters between Pu(III) and Cl^-, as well as the standard chemical potential for Pu(OH)3(s). The ion interaction parameters are given in Table 14; these are assumed to apply equally well to Am(III) by analogy. The standard chemical potential for Pu(OH)3(s) is converted to that for Am(OH)3(s) in Table 15.

Rao et al. (1994) parameterized ion interactions for Nd(III) in concentrated $NaHCO_3$ and Na_2CO_3 media, extending the work for Felmy et al. (1990) to the large carbonate concentrations that could occur in WIPP under disposal scenarios with large CO_2(g) pressures. They identified an additional Nd(III) solid phase that forms under concentrated conditions, and had to modify one of the ion interaction parameters determined in Felmy et al. (1990). The parameters from Rao et al. (1994), converted to apply to Am(III) species, are given in Tables 16 and 17.

Interactions for Nd(III) or Am(III) with phosphate species are discussed in Rai et al. (1992a, 1992b) and Rai et al. (1994). These papers present the standard chemical potentials for H_3PO_4, $H_2PO_4^-$, HPO_4^{2-}, and PO_4^{3-}, as shown in Table 18. The reported standard chemical potentials for

H_3PO_4 and $H_2PO_4^-$, taken from Pitzer and Silvester (1976) as the original source, are the same. However, there are slight differences in the standard chemical potentials given for HPO_4^{2-}, and PO_4^{3-}, even though these are all reported as having been taken from Wagman et al. (1982). The differences in these reported values are slight and will have no significant impact on calculations using these numbers. We have gone back to the original Wagman et al. (1982) reference to arrive at the selected values indicated in Table 18. Ion interaction parameters for phosphoric acid, taken from Pitzer and Silvester (1976), are given in Table 19.

The standard chemical potentials for three different Am(III)-phosphate or analogous Nd(III)-phosphate phases are reported in Rai et al. (1992a, 1992b) and Rai et al. (1994). These values, along with conversion from Nd(III) to Am(III) where necessary, are given in Table 20. The difference among the calculated values for the standard chemical potentials for the americium phosphate solid phase is less than 0.9 units; all values are effectively the same. However, because the value from Rai et al. (1992a) was determined for Am directly, not for Nd, this value was selected for use in HMW_NP_AM.CHEMDAT.

Table 21 contains the ion interaction parameters developed for Nd(III) or Am(III) in Rai et al. (1994). The publication of Novak et al. (1995) provides a comprehensive description of the sources for and the rationale for selection of the Am(III) thermodynamic parameters that will be incorporated into future versions of the CHEMDAT file.

Table 8. Ion interaction parameters from Pitzer (1991), converted to values needed for FMT.

1-1 electrolytes	$\beta^{(0)}$	$\beta^{(1)}$	$C\phi$
Na^+-ClO_4^-	0.0554	0.2755	–0.00118
Na^+-$H_2PO_4^-$	–0.0533	0.0396	0.00795
K^+-$H_2PO_4^-$	–0.0678	–0.1042	0
H^+-ClO_4^-	0.1747	0.2931	0.00819

2-1 electrolytes	$\frac{4}{3}\beta^{(0)}$	$\frac{4}{3}\beta^{(1)}$	$\frac{2^{5/2}}{3}C^{\phi}$	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}
Na^{+}-HPO_4^{2-}	–0.0777	1.954	0.0554	–0.0583	1.466	0.0294
K^{+}-HPO_4^{2-}	0.0330	1.699	0.0309	0.0248	1.274	0.0164
Ca^{2+}-ClO_4^{-}	0.6015	2.342	–0.00943	0.4511	1.756	–0.00500
Mg^{2+}-ClO_4^{-}	0.6615	2.678	0.01806	0.4961	2.008	0.009578
UO_2^{2+}-Cl^{-}	0.5698	2.192	–0.06951	0.4274	1.644	–0.03686
UO_2^{2+}-ClO_4^{-}	0.8151	2.859	0.04089	0.6113	2.144	0.02168

3-1 electrolytes	$\frac{3}{2}\beta^{(0)}$	$\frac{3}{2}\beta^{(1)}$	$\frac{3^{3/2}}{2}C^{\phi}$	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}
Na^{+}-PO_4^{3-}	0.2672	5.777	–0.1339	0.1781	3.851	–0.05154
K^{+}-PO_4^{3-}	0.5594	5.958	–0.2255	0.3729	3.972	–0.08680

2-2 electrolytes	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}
UO_2^{2+}-SO_4^{2-}	0.322	1.827	–0.0176

Table 9. Standard chemical potentials for neptunyl(V) species, from Novak and Roberts (1995).

Species	μ_f^o/RT	Species	μ_f^o/RT
NpO_2^+	–369.127	$NaNpO_2CO_3(s)$	–713.707
$NpO_2OH(am)$	–452.642	$NpO_2CO_3^-$	–594.492
$NpO_2OH(aged)$	–454.010	$NpO_2(CO_3)_2^{3-}$	–808.403
$NpO_2OH(aq)$	–438.518	$NpO_2(CO_3)_3^{5-}$	–1019.918
$NpO_2(OH)_2^-$	–505.829		

Table 10. Ion interaction parameters for neptunyl(V) species, from Novak and Roberts (1995).

$^{(0)}\beta_{NpO_2^+-ClO_4^-}$	0.312	$^{(0)}\beta_{Na^+-NpO_2CO_3^-}$	0.161	β\s((0),Na^+-$NpO_2(CO_3)_3^{5-}$)	1.97
$^{(0)}\beta_{NpO_2^+-Cl^-}$	0.169	β\s((0),Na^+-$NpO_2(CO_3)_2^{3-}$)	0.407	β\s((1),Na^+-$NpO_2(CO_3)_3^{5-}$)	16

Table 11. Dimensionless standard chemical potentials for Am(III) species from Felmy et al. (1990)

Species	μ_i^o / RT
Am^{3+}	–241.694
$AmCO_3^+$	–472.06
$Am(CO_3)_2^-$	–695.88
$Am(CO_3)_3^{3-}$	–915.46
AmOHCO3(c)	–569.98

Table 12. Specific ion interaction parameters for Am(III) species from Felmy et al. (1990).

	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^{ϕ}
Na^{+} - ClO_4^{-}	0.80	5.35	0	–0.0048
Na^{+} - $Am(CO_3)_3^{3-}$	0.24*	8.1	0	0

* this value is modified in Table 17

Table 13. Dimensionless standard chemical potentials for Nd(III) species from Rai et al. (1992b), with calculated values for analogous Am(III) species.

Nd Species	μ_i^o / RT	Am Species	μ_i^o / RT
Nd^{3+}	–270.926	Am^{3+}	–241.694
$Nd(OH)_2^{+}$	–422.879	$Am(OH)_2^{+}$	–393.647*
$Nd(OH)_3^{0}$	–492.182	$Am(OH)_3^{0}$	–462.950*
$Nd(OH)_3(gl)$	–527.259	$Am(OH)_3(gl)$	–498.027*

*calculated by equation 17

Table 14. Specific ion interaction parameters for Am(III) species from Felmy et al. (1989), and, by analogy, for Am(III).

	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^{ϕ}
Pu^{+++} - Cl^{-}	0.6117	5.403	0	–0.0284
Am^{+++} - Cl^{-}	0.6117	5.403	0	–0.0284

Table 15. Dimensionless standard chemical potentials for Pu(III) species from Felmy et al. (1989), with calculated values for analogous Am(III) species.

Pu Species	μ_i^o / RT	Am Species	μ_i^o / RT
Pu^{3+}	–233.4	Am^{3+}	–241.694
$Pu(OH)_3(s)$	–484.0	$Am(OH)_3(s)$	–492.294*

*calculated by equation 17

Table 16. Dimensionless standard chemical potentials for Nd(III) species from Rao et al. (1994), with calculated values for analogous Am(III) species.

Nd Species	μ_i^o / RT	Am Species	μ_i^o / RT
Nd^{3+}	–270.926	Am^{3+}	–241.694
$NaNd(CO_3)_2 \cdot 6H_2O(c)$	–1425.726	$NaAm(CO_3)_2 \cdot 6H_2O(c)$	–1396.494*

*calculated by equation 17

Table 17. Specific ion interaction parameters for Nd(III) species from Rao et al. (1994), and, by analogy, for Am(III).

	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^ϕ
$Na^+ - Nd(CO_3)_2^-$	0	–8.37	0	0
$Na^+ - Nd(CO_3)_3^{3-}$	–0.94*	8.1	0	0.418
$Na^+ - Am(CO_3)_2^-$	0	–8.37	0	0
$Na^+ - Am(CO_3)_3^{3-}$	–0.94*	8.1	0	0.418

*this value was changed from that given in Felmy et al. (1990)

Table 18. Standard chemical potentials for phosphate species, with selected values for HMW_NP_AM.CHEMDAT data base.

name	Rai et al. (1992a)	Rai et al. (1992b)	Rai et al. (1994)	selected value
$H_3PO_4(aq)$	–460.90	–460.90	–460.90	–460.90
$H_2PO_4^-$	–455.96	–455.960	–455.960	–455.960
HPO_4^{2-}	–439.404	–439.354	–439.354	–439.367
PO_4^{3-}	–410.98	–410.947	–410.947	–410.947

Table 19. Specific ion interaction parameters for $H_3PO_4(aq)$ from Pitzer and Silvester (1976).

	λ
H^+ - $H_3PO_4(aq)$	0.290
K^+ - $H_3PO_4(aq)$	–0.070
HPO_4^{2-} - $H_3PO_4(aq)$	–0.400

Table 20. Standard chemical potentials for Am(III)- or Nd(III)-phosphate solid phases.

Nd Solid Phase	μ_i^o / RT	Am Solid Phase	μ_i^o / RT
Nd^{3+}	–270.926	Am^{3+}	–241.694
		AmPO4•xH2O(am), Rai et al. (1992a)	–709.75
NdPO4(c), Rai et al. (1992b)	–738.166	AmPO4(c)	–708.934*
NdPO4(c), Rai et al. (1994)	–738.63	AmPO4(c)	–709.398•

*calculated by equation 17

Table 21. Specific ion interaction parameters for Nd(III) species from Rai et al. (1994), and, by analogy, for Am(III).

	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^{ϕ}
$Nd^{3+} - SO_4^{2-}$	3.0398	0	–2500	0
$Nd^{3+} - H2PO_4^{-}$	0	0	–92.9	0
$Am^{3+} - SO_4^{2-}$	3.0398	0	–2500	0
$Am^{3+} - H2PO_4^{-}$	0	0	–92.9	0

7.3.3 Description of HMW_NP_AM.CHEMDAT

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 a line shown in the listing of HMW_NP_AM.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.

Some of the standard chemical potentials for species, i.e., lines 39-49 and 70-72 in Appendix I, are described as "arbitrary." The Table 22 lists the value, the lines where instances occurred, and the definition of the value.

Table 22. Arbitrary values used for standard chemical potentials

Arbitrary Values	**Example in Lines**	**Definition**
–999.99	39, 40, 70, 72	physical species but represent the only occurrence for that element that have no chemical reactions in solution
0	45, 46, 49	nonphysical species that are 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 and are 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. They facilitate, e.g., addition of HCl(aq) to adjust the pH, insuring complete dissociation. To make sure these species are never calculated as being present, they were arbitrarily assigned the large positive value 500 for dimensionless standard chemical potential.

In Table 23 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 23. CHEMDAT input parameters (Listing of HMW_NP_AM.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, 3=gas, but gasses are unsupported); standard chemical potential of the species (in the units indicated by the flag in line 6). Entries in the formula vector usually are, but need not be, integers, and can be positive or negative. H_2O must always be the first species declared. All aqueous species must be declared before any solid species is declared.
142	DUMMY2, ITEMP	character flag that, when set to 'DG_BYPASS' allows alternate values for the standard chemical potentials to be read from file "bypass" for the first ITEMP species.
143	DUMMY2	character flag that enables the use of the Pitzer activity coefficient model when equal to 'PITZACT'. Any other character string will disable the Pitzer activity coefficient model.
144	NCATION	number of cations for which Pitzer activity coefficient model is used (positive integer) See note below Line 855 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	ELMAP(1,i)	maps the location in the species list to the order the Pitzer parameters were entered: cation map
854	ELMAP(2,i)	anion map
855	ELMAP(3,i)	neutral species map

		Note on species order: cationic, anionic, and neutral species are referenced by the order given in ELMAP(,). This is determined as follows: the cations are the second, third, fourth, fifth, sixth, seventh, twenty-second, etc., species entered in the species list, i.e., Na+, K+, Ca+, Mg+, MgOH+, H+, $MgB(OH)_4^+$, etc. Similar patterns are used for anions and cations. This allows additional flexibility in reorganizing and rearranging the data input files without having to reenter all of the ion interaction parameters. Although the order is arbitrary, it is very important that a consistent order is maintained throughout the CHEMDAT file. Because all parameters are clearly labeled, the echo printing of the ion interaction parameters makes is easy to determine whether errors were made when changing the CHEMDAT file. *****CAUTION***** **THE USER SHOULD NOT ALTER THE CHEMDAT FILE.**
857	DUMMY, NEQACT	character flag that, when equal to 'EQUALACT', indicates that NEQACT (positive integer) activity coefficients of "nonPitzer" species will be set equal to activity coefficients of Pitzer species. For example, one could run calculations using both 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.
859	RPLWCHG	positive integer indicating the element to RePLace With CHarGe. Used to implement the constraint of solution charge neutrality. The 2nd element corresponds to oxygen.
860	DUMMY, NEHRXN	character flag indicating whether redox reactions are specified (they are when the flag is 'REDOX'). When this flag is used, it will be followed by specifications of NEHRXN (positive integer) redox reactions. This feature is unsupported in FMT V2.0.
861	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 V2.0.

7.3.4 Description of OUTPUT File "BATCH.DOC" for HMW_NP_AM.CHEMDAT

The output file "BATCH_DOC.OUT," provided in Appendix J, is used to illustrate the lines echoing the CHEMDAT file. Table 24 explains this file. The OUTPUT file for a titrate problem will have an extra 5 lines after line 1277. The additional lines are described on line 1277 of Table 24. Line 1280 for the batch problem would be line 1285 for a titrate problem.

Table 24. OUTPUT file description of CHEMDAT input parameters (See listing provided in Appendix J.)

Line	Variable Name	Description
1		notation; FMT sets temperature to 298.15 Kelvin
2	TITLE99	problem title specified on line 1 of INPUT file with 'FMT' and version number appended
3-4	DBASE1, DBASE2	unique identification specified on lines 1 and 2 of CHEMDAT file
6	ACCURCY	convergence tolerance for equilibrium calculations, specified on line 5 of CHEMDAT file
7	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).
8	NAQ	number of aqueous species in CHEMDAT
11		notation; species listed in order for Pitzer parameters
13-18	NAMES (ELMAP(1,i))	ordered list of cation species
20-26	NAMES (ELMAP(2,i))	ordered list of anion species
29-32	NAMES (ELMAP(3,i))	ordered list of neutral species
34-296		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 23, lines 148-419)
298-338		table of cation-cation ternary interactions and parameters
	NAMES (ELMAP(1,j))	up to 10 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 15-18
	ME(i,j,1)	cation-cation ternary interaction parameter, θ_{ij}
341-416		table of anion-anion ternary interaction and parameters
	NAMES (ELMAP(2,j))	up to 10 columns of anion names on a line after leading anion
	NAMES (ELMAP(2,i))	name of leading i^{th} anion on ordered list
	ME(i,j,1)	anion-anion ternary interaction parameters, θ_{ij}
419-579		table of cation-cation-anion ternary interaction and parameters
	NAMES (ELMAP(2,k))	up to 10 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}
581-965		table of anion-anion-cation ternary interaction and parameters

	NAMES (ELMAP(1,k))	up to 10 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}
967-982		table of neutral-cation binary interaction and parameters
	NAMES (ELMAP(3,i))	up to 10 columns of neutral species names on a line
	NAMES (ELMAP(1,j)), NEUCAT(i,j)	j^{th} cation name and up to 10 binary interaction values, λ_{ij}
985-1007		table of neutral-anion binary interaction and parameters
	NAMES (ELMAP(3,i))	up to 10 columns of neutral species names on a line
	NAMES (ELMAP(2,j)), NEUANI(i,j)	j^{th} anion name and up to 10 binary interaction values, λ_{ij}
		table of neutral-cation-anion ternary interaction and parameters
1009-1272	NAMES (ELMAP(3,i))	up to 10 neutral species names in columns on a line
	NAMES (ELMAP(1,j)), NAMES (ELMAP(2,k))	j^{th} cation and k^{th} anion names
	PTZTSI(i,j,k)	up to 10 ternary interaction values, ζ_{ijk}
1273		notation that Pitzer activity coefficient model is used
1274	ELNAME (RPLWCHG)	states name of element replaced by charge balance (see Table 23, line 859)
1277		notation that the problem is BATCH (If this were a titration problem, notation would be that the problem is TITRATION.)

	CDUM1,CDUM2	5 extra lines for a TITRATION problem: notation defining delta(x) echoing character flags set by INPUT file in line 64 Note: Line count will be off by +5 for titrate problems
1280		notation that FMT uses dimensionless gas constant
1281	TKELVIN	temperature in degrees Kelvin, same as TEMPERA
1284	ALLSPEC, TTLELEM	number of species, number of elements
1286- 1309	ELNAMES(i), MWELEM(i)	name and molecular weight of i^{th} element
1312- 1427		listing of each species' chemical properties
	i, NAMES(i)	number and name of i^{th} chemical species
	PSNAME (PHASE(i))	string notation for the phase of the i^{th} species
	MWSPEC(i)	molecular weight of i^{th} species; computed as: ΣFORMULA(j,i)*MWELEM(j), where FORMULA(j,i) is the stoichiometric number of j^{th} element in the i^{th} species, MWELEM(j) is the molecular weight of the j^{th} element, index j runs through all elements, and index i runs through all species
	MU0FORM(i)	standard chemical potential of the i^{th} species
1430- 1545		table showing relationship of species to elements
	i,NAMES(i)	number and name of i^{th} chemical species
	FORMULA(j,i), j=1,ttlelem	stoichiometric number of each element in the i^{th} species

7.4 Standard RHOMIN Input File

The input file RHOMIN, another data base, 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.RHOMIN, contains mineral densities in units of kg/m^3 or equivalently in g/L, $\rho_{MINERALS}$, for all of the minerals contained in the CHEMDAT file. The numerical values for mineral densities were taken from Weast (1980) when available, otherwise the minerals were arbitrarily assigned a value of 2000 g/L. Mineral densities are not needed to calculate the chemical equilibrium problems that FMT 2.0 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 2.0 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 from the next extensive 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 25, which describes the input parameters for HMW_NP_AM.RHOMIN, the "Variable Name" column is for the FMT program variables. FMT reads only the number on each line of HMW_NP.RHOMIN. The species name on the line is for human readability and is not read by FMT.

Table 25. RHOMIN input parameters (See Appendix K for listing, and Appendix L for output file 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 is also described after the section on fatal error messages.

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* that is usually defaulted 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 ...' indicate that the run time value in FMT will be listed.

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

8.1.1 "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
**************************************
```

8.1.1.1 Explanation

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:

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

* 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.

- "INITIAL," the second or titrated solution does not have a zero charge balance

8.1.1.2 Suggested Solution

Change the charge amount in the INPUT file to zero.

8.1.2 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
**************************************
```

8.1.2.1 Explanation

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

8.1.2.2 Suggested Solution

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

8.1.3.1 Explanation

The initial guess routine could not find an estimated solution for the given input. The initial guess 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.

8.1.3.2 Suggested 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. The objective is to develop a reasonable set of species values to give to the initial guess algorithm.

8.1.4 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
**************************************
```

8.1.4.1 Explanation

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.

8.1.4.2 Suggested Solution

Contact the code sponsors. This message indicates programming errors.

8.1.5 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
**************************************
```

8.1.5.1 Explanation

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

8.1.5.2 Suggested Solution

Contact the code sponsors to set a higher limit for MAXELEM.

8.1.6 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
**************************************
```

8.1.6.1 Explanation

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.

8.1.6.2 Suggested Solution

Contact the code sponsors to set a higher limit for MAXSPEC.

8.1.7 MUST PUT ALL AQUEOUS . . .

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

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

8.1.7.1 Explanation

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

8.1.7.2 Suggested Solution

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

8.1.8 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
**************************************
```

8.1.8.1 Explanation

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 FMT2P0", 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 amount for a titrated solution could be essentially zero which is less than -1.0×10^{-12}.

The other 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

8.1.8.2 Suggested Solution

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 NEW T" option . . .

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

8.1.9.1 Explanation

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

8.1.9.2 Suggested Solution

Notify the code sponsors and change the character string to 'nNEW T' in CHEMDAT.

8.1.10 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)'
**************************************
```

8.1.10.1 Explanation

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).

8.1.10.2 Suggested Solution

Contact the code sponsors. The algorithm has checked at least 20 different sets of solids and found no equilibrium solution. Either the problem is incredibly 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.

8.1.11 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'
*************************************
```

8.1.11.1 Explanation

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

8.1.11.2 Suggested Solution

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 Species "H2O" must be first . . .

Reduce the NSPACE parameter in the INPUT file to 66 or less.

```
*************************************
[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
*************************************
```

8.1.12.1 Explanation

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 Appendix I listing of HMW_NP_AM.CHEMDAT.

8.1.12.2 Suggested Solution

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

8.1.13 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.
*************************************
```

8.1.13.1 Explanation

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 5).

8.1.13.2 Suggested Solution

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

8.1.14.1 Explanation

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).

8.1.14.2 Suggested Solution

Increase the amounts of elements in the INPUT file or amounts of species in the INGUESS file.

8.1.15 VALID CHARGE BALANCE ELEMENT NOT . . .

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

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

8.1.15.1 Explanation

This error occurs in the CHEMDAT file when the variable RPLWCHG is negative or zero. The RPLWCHG variable is read on line 859 as a 2 (the element Oxygen) in Appendix I listing of HMW_NP_AM.CHEMDAT.

8.1.15.2 Suggested Solution

Notify the code sponsors.

8.1.16 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.
**************************************
```

8.1.16.1 Explanation

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 5).

8.1.16.2 Suggested Solution

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. The water is used up 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. A suggested solution is to increase the amount of water to the INGUESS file or decrease species amounts.

8.3 Warning Messages

There are warning messages that indicate the solution is not a valid one.

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 BATCH CALCULATION ERRORS . . .

```
**************************************
[on unit 6]
BATCH CALCULATION ERRORS, L2 norm 'value for L2 norm'
SEE OUTPUT FOR MASS BALANCE ERROR INSTRUCTIONS

[in OUTPUT file]
BATCH CALCULATION ERRORS, L2 norm 'value for L2 norm'
{a listing of the initial and final abundances, element names and the absolute
value of the differences between the initial and final abundances}
MASS BALANCE ERROR INSTRUCTIONS
```

```
1) Check to see how much abundances have changed
   Should only happen in batch problems, or when
   flashing initial or injected conditions

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

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

8.3.1.1 Explanation

This message warns that material balance errors are present during the flash calculation. This message occurs when material and charge balances exceed 1.0×10^{-6}. FMT prints the above message and continues on to the next flash in a titration problem.

8.3.1.2 Suggested Solution

None, but answer (if any) is invalid.

8.3.2 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
**************************************
```

8.3.2.1 Explanation

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 HMW_NP_AM.CHEMDAT has 115 species.

8.3.2.2 Suggested Solution

Verify that H+ species is not in the CHEMDAT file and notify the code sponsors.

8.3.3 "EXACT" mole amounts . . .

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

8.3.3.1 Explanation

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.

8.3.3.2 Suggested Solution

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 MASS BALANCE ERRORS . . .

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

8.3.4.1 Explanation

This message warns that material balance errors were detected during the flash calculation. FMT prints the above message and continues to the next Erlenmeyer solution in a titration problem.

8.3.4.2 Suggested Solution

None, but answer (if any) is invalid.

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 occurs in a batch problem when the mu value or concentration of aqueous/sorbed species exceeds 1.0×10-24 as specified by minabu×1.0×10-6, the convergence tolerance read from CHEMDAT. This message refers to FMT's normal algorithmic attempts to adjust the stoichiometric equation for the lack of species. These messages appear during execution of a batch problem as indicators of normal computational progress.

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 chemical reactions to equilibrate, which by definition means the system is at equilibrium.

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.

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 mu value or concentration of a solid species exceeds 1.0×10^{-6} as specified by accuracy, the convergence tolerance read from CHEMDAT. This message refers to FMT's normal algorithmic attempts to adjust the stoichiometric equation for the lack of species.

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 a solid species needs to be included in a solution. A count of the number of solubility violations found during the equilibrium process. The largest mu value of a solid species is listed.

8.4.6 Switching Routine Hung . . .

```
**************************************
[on unit 6]
Switching Routine Hung, Ending Batch Calculation
*** Flash Calculation Terminated ***
***   Infinite Loop Encountered  ***
*** spacepoint='value of Erlenmeyer solution'

[in OUTPUT file]
Flash-Terminated (sp) 'value of Erlenmeyer solution'
*** Flash Calculation Terminated ***
***   Infinite Loop Encountered  ***
*** spacepoint= 'value of Erlenmeyer solution'
**************************************
```

A species has a calculated concentration right on the border 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^{-22}), this message has no consequences unless the user is looking at very trace species.

9.0 DESCRIPTION OF OUTPUT FILES

FMT generates a primary OUTPUT (.OUT) file and the secondary output files shown in Figures 1 and 2. Secondary output files vary according the 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 and MOLES are the secondary files 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 26 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 26. OUTPUT File Description for Batch (See Appendix M for sample listing.)

Line	Variable Name	Description
1	INFNM	INPUT filename.
2	INGFNM	INGUESS filename.
3	OUFNM	OUTPUT filename.
4	CHFNM	CHEMDAT filename.
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

11-14		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.
17-25		this section contains computation status indicators printed during calculations to find the equilibrium system.
17-21	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.
23	NKSPVIO	number of solubility product violations for solids (minerals)
24	NAMES(i)	postulated that brucite was present in the equilibrium system, and thus added to the equilibrium calculations
25	ALLITER	number of times the diagonalized Hessian matrix system of equations was solved to reach the calculated equilibrium state
26		Note: a page break occurs; the first character "1" indicates a Fortran page break and is deleted before printing the remaining line
26-28	TITLE99, DBASE1, DBASE2	problem title and CHEMDAT input file (Appendix I) identification
29	PRESSUR, TEMPERA	pressure and temperature for batch problem
31-58		table of Elemental Abundances
	ABUND(i)	"Total Moles" column contains the exact number of moles for each element as read from the INPUT file, or as calculated from species abundances as read from the INGUESS file
	AQMOLES(i)/ KGH2O	"Aq. Molality" column is the total molality for each element in the aqueous phase
	AQMOLES(i)/ SOLNVOL	"Aq. Molarity" column is the total molarity for each element in the aqueous phase. This number is calculated from the solution density, as discussed on lines 54-67.
	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

60-73		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 35) to calculate solution density from total dissolved solids (TDS).
61-63	SOLMASS, KGH2O×1000, TDSGPKG	values calculated from equilibrium compositions
66	SPRHO	density specified in the INPUT file for titrate problems. For BATCH problems the solution density from the NaCl correlation is automatically used.
69-70	SOLNVOL, TDS	calculated values based on specified density on line 66
72	DENSITY(2, TDSGPKG)	density calculated by FMT using the NaCl correlation
73	(DENSITY(2, TDSGPKG)/ SPRHO-1.)×100	difference between the specified density (line 66) and the density calculated by FMT which will always be zero for BATCH problems
77-161		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 56 is zero, so no detailed information is given for phosphorus species.
	NAMES(i)	"Species Name" column
	MOLALTY(i) or for solids: NMOLES(i)/ NMOLES(1)/ MWH2O	"Molality" column contains the species molality, moles per kg H_2O, for all species including solids. However, the entry for water is not molality of water, which is invariant, but the mole fraction H_2O in the aqueous phase, as noted on line 170.
	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 60-73

	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 172-176
163	-(NMOLES (NPROTON)/ NMOLES(1)/ MWH2O)	pmH: the negative base 10 logarithm of hydrogen ion molality
164	PHVECT	pH: the negative base 10 logarithm of hydrogen ion activity
165	OSM	osmotic coefficient, a value related to the activity of water; a value calculated from the Pitzer equations
166	LNGAMA(1)×100	equilibrium relative humidity, equal to 100% times the water activity
167	IONICST	ionic strength, in molal units, defined as $\sum_{i=2}^{Nspec} z_i^2 m_i$, where z_i is the charge on the i^{th} species, m_i is the molality of the i^{th} species, and index i runs from species 2 through all aqueous species, with species 1 defined as H_2O
168	SPRHO	solution density, calculated as described on lines 60-73
170-171		*notes defining water and gas molality*
172-176		notes describing the descriptor column in table of concentrations for batch system
178	ΣCHEMPOT(i)× NMOLES(i)	the total dimensionless Gibbs free energy for the solution; the quantity that is minimized to find the equilibrium composition
180	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 25
181	ICNT	number of times the species list was changed for computational purposes in the minimization algorithm

In the BATCH_DOC.OUT file on lines 31-58, the first table gives the elemental abundances in various units, the first column being the number of total moles, and the second being the aqueous molality. The "Total Moles" column 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 "Aq. Molality" column given 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.

Lines 77-161 which comprise the second table, Table of Concentrations for Batch System, list 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 6 of the output file listing for the CHEMDAT file; see Appendix J). The *component* species, lines 81-90, 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 91-101, all have absolute values less than 10^{-6}, thus indicating convergence. The remaining species, lines 102-161, 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 175 indicates, the descriptor value for aqueous species with zero concentrations is approximately equal to the $\log_{10}$ concentration of that aqueous species in this solution. (For comparison, one atom in 1 kg H_2O would have a molal concentration of 1.6×10^{-24} molal, corresponding to a descriptor value of –23.8.) These values are a consequence of the choice of values for the standard chemical potentials of these species. As discussed in the CHEMDAT data base documentation (Section 7.3 and Appendices I and J), these species are nonphysical and included for convenience only.

9.1.2 Titrate Problem

Table 27 explains the printout for a titrate problem using the OUTPUT file generated from executing Np_NaCl_BM_LOG. (It also explains the printout of the OUTPUT file generated from executing 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 27. OUTPUT File Description for Titrate (See Appendices N, O, and P 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 filname
2	INGFNM	INGUESS filname
3	OUFNM	OUTPUT filname
4	CHFNM	CHEMDAT filname
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
11-14		this location would normally be filled with an echo print of ion interaction parameters and chemical species definitions, as read from the CHEMDAT. This information is reproduced in the OUTPUT file listing provided in Appendix J and is described therein.
17-20		notation of parameters set for fracture/matrix transport
24		notation of porosity
27		notation of aqueous density
29	RHFNM	RHOMIN filename
31-34		this location would normally be filled with an echo print of mineral species and their densities, as read from RHOMIN. This information is reproduced in the OUTPUT file listing provided in Appendix L and is described therein.
36-44	GBV(i)	unused 3 sets of grid blocks in fracture/matrix transport each containing N_S solutions
46-139		summary information for the titrant solution flash calculation
140-237		summary information for the Erlenmeyer solution flash calculation
238		notation; first beaker of Erlenmeyer solution

238-336		summary information for the first beaker (same as Erlenmeyer solution when corrected for different volumes)
337		notation; second beaker of Erlenmeyer solution
337-435		summary information for addition of DV(2)* to 1 liter of the Erlenmeyer solution
436		notation; third beaker of Erlenmeyer solution
436-534		summary information for addition of DV(3)* to 1 liter of the Erlenmeyer solution
535		notation; fourth beaker of Erlenmeyer solution
535-633		summary information for addition of DV(4)* to 1 liter of the Erlenmeyer solution
634		notation; fifth beaker of Erlenmeyer solution
634-732		summary information for addition of DV(5)* to 1 liter of the Erlenmeyer solution
733		notation; sixth beaker of Erlenmeyer solution
733-831		summary information for addition of DV(6)* to 1 liter of the Erlenmeyer solution
832		notation; seventh beaker of Erlenmeyer solution
832-930		summary information for addition of DV(7)* to 1 liter of the Erlenmeyer solution
931		notation; eighth beaker of Erlenmeyer solution
931-1029		summary information for addition of DV(8)* to 1 liter of the Erlenmeyer solution
1030		notation; ninth beaker of Erlenmeyer solution
1030-1128		summary information for addition of DV(9)* to 1 liter of the Erlenmeyer solution

* Summary information for DV(2) through DV(14) not shown in listings for Np_NaCl_BM_LIN.OUT and Np_NaCl_BM.OUT.

1129		notation; 10th beaker of Erlenmeyer solution
1129-1227		summary information for addition of *DV(10)** to 1 liter of the Erlenmeyer solution
1228		notation; 11th beaker of Erlenmeyer solution
1228-1326		summary information for addition of DV(11)* to 1 liter of the Erlenmeyer solution
1327		notation; 12th beaker of Erlenmeyer solution
1327-1425		summary information for addition of DV(12)* to 1 liter of the Erlenmeyer solution
1426		notation; 13th beaker of Erlenmeyer solution
1426-1524		summary information for addition of DV(13)* to 1 liter of the Erlenmeyer solution
1525		notation; 14th beaker of Erlenmeyer solution
1525-1623		summary information for addition of DV(14)* to 1 liter of the Erlenmeyer solution
1624		notation; 15th (last) beaker of Erlenmeyer solution
1624-1722		summary information for addition of DV(15)** to 1 liter of the Erlenmeyer solution
1723	TIFNM	TITRATE filename***
1724	MOFNM	MOLES filename****

** Summary information for DV(15) in listings for Np_NaCl_BM_LIN.OUT and Np_NaCl_BM.OUT are from lines 343-441.

*** On line 442 in listings for Np_NaCl_BM_LIN.OUT and Np_NaCl_BM.OUT.

**** On line 443 in listings for Np_NaCl_BM_LIN.OUT and Np_NaCl_BM.OUT.

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 28 explains the FOR088 file generated from a batch problem. The "Line" column refers to the line numbers listed in BATCH_DOC.FOR088.

Table 28. FOR088 File Description for Batch (See Appendix Q for sample listing.)

Line	Variable Name	Description
1-115	NMOLES(i)	total number of moles for the i^{th} species
	NAMES(i)	the i^{th} species names
	NMOLES(i)/ NMOLES(1)/ MWH2O	the i^{th} species molality, moles per kg H_2O (see line 77-161 "Molality" column in Table 26 and Appendix M)

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 29 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 S and T, respectively.

Table 29. TITRATE File Description (Appendix R)

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	NAMES(i)	table of all species molal concentrations
		up to 9 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
	EH(j)	the Eh (an option which is not supported in FMT 2.0)
	DV(j)*1.d3	titrant volume
	PHVECT(j)	pH of solution

9.4 MOLES

The titrate secondary output files are TITRATE and MOLES.

Available for diagnostic purpose, the MOLES file, a secondary output file for the titrate problem, contains the equilibrated concentrations of the initial solution. The MOLES file should be deleted after each execution of FMT.

Table 30 describes a MOLES file generated by FMT. The "Line" column refers to the line numbers listed in Np_NaCl_BM_LOG.MOLES. (No printouts for Np_NaCl_BM_LIN.MOLES and Np_NaCl_BM.MOLES are appended to this manual.)

Table 30. MOLES File Description (See Appendix U for sample listing of Np_NaCl_BM_LIN.MOLES.)

Line	Variable Name	Description
1-3	TITLE99, DBASE1, DBASE2	problem title and CHEMDAT identification
5-28	ELNAMES(i), ELTOTAL(i,1), ELTOTAL(i,2)	listing of the elements, elemental abundances for injected solution (buret) and initial solution (Erlenmeyer) as read from the INPUT file
30-53	ELNAMES(i), ELTOTAL(i,1), ELTOTAL(i,2)	after reading the INGUESS file for species abundances, if requested, and equilibrating both solutions the listing of elements, elemental abundances of the injected solution and the initial solution before any titration begins

55-170	NAMES(i), IJCONCS(i,1), IJCONCS(i,2)	listing of the species, the injected concentrations and the initial concentrations

10.0 REFERENCES

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Novak, C.F., and K.E. Roberts. 1995. "Thermodynamic Modeling of Neptunium(V) Solubility in $Na\text{-}CO_3\text{-}HCO_3\text{-}Cl\text{-}ClO_4\text{-}H\text{-}OH\text{-}H_2O$ Electrolytes," *Materials Research Society Symposium Proceedings, Volume 353. International Symposium on the Scientific Basis for Nuclear Waste Management (18th: 1994: Kyoto, Japan).* pp. 1119-1128.

Novak, C.F., C.C. Craft, and N.J. Dhooge. 1995. *Thermodynamic modeling of +III Actinide solubility in concentrated Na-Cl-SO4-CO3-PO4 electrolytes: predicted phase diagrams and comparison with experiment.* SAND95-0258. Albuquerque, New Mexico: Sandia National Laboratories.

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

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

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

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

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

Rao, L., D. Rai, A.R. Felmy, and RW. Fulton. 1994. "Solubility of $NaNd(CO_3)_2 \cdot 6H_2O$ in Concentrated Sodium Carbonate and Sodium Bicarbonate Solutions." *Radiochimica Acta* vol. ___: ___-___. SAND94-1948J.

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

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

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

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

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

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

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

11.0 APPENDICES

Note

The numbers to the left of each line in Appendices A through U 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 U are examples *only*. They *are not* necessarily representative of files used to support the 1996 WIPP PA regulatory calculation.

Appendix A: Sample Screen Display of BATCH_DOC

See Table 1 for explanation of this screen display.

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

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.CHEMDAT "Initial load"
FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
Select CHEMDAT name from list above: FMT_HMW_NP_AM.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.CHEMDAT fetched

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.RHOMIN "Initial load"
Select RHOMIN name from list above: FMT_HMW_NP_AM.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.RHOMIN fetched

                image name: "FMT_FMT2P0"
                image file identification: "PROD PA96"
                image file build identification: ""
                link date/time: 21-DEC-1995 11:36:28.86
                linker identification: "A11-14"

Entering Subroutine READDAT
reading chemical species data from CHEMDAT file
DG_BYPASS flag set to nDG_BYPASS
[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs                FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,F91,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
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

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

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

Appendix A: Sample Screen Display of BATCH_DOC

```
.LT. (MINABU*1.d-6) moles K8H6(SO4)7_____Misenite; del&reopt
.LT. (MINABU*1.d-6) moles K8H4(CO3)6.3H2O___K-Sequicarbonate; del&switch
.LT. (MINABU*1.d-6) moles B3O3(OH)4-          B3O3(OH)4-; del&switch
.LT. (MINABU*1.d-6) moles Ca4Cl2(OH)6.13H2O__CaOxychloride A; del&switch

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

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

          2 Solubility Product Violations
Adding solid Mg(OH)2_____Brucite
pmH = -log[m(H+)]                =     12.7140
pH = -log[a(H+)]     =     12.8532
Total Diagonal Inversions          85
Total Stoichiometric Reoptimizations          10
SINGLE BATCH EQUILIBRATION COMPLETED
```

Appendix B: Sample Screen Display of Np_NaCl_BM_LOG

See Table 3 for explanation of this screen display.

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

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.CHEMDAT "Initial load"
FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
Select CHEMDAT name from list above: FMT_HMW_NP_AM.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.CHEMDAT fetched

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.RHOMIN "Initial load"
Select RHOMIN name from list above: FMT_HMW_NP_AM.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.RHOMIN fetched

                image name: "FMT_FMT2P0"
                image file identification: "FROD PA96"
                image file build identification: ""
                link date/time: 21-DEC-1995 11:36:28.86
                linker identification: "A11-14"

Entering Subroutine READDAT
reading chemical species data from CHEMDAT file
DG_BYPASS flag set to nDG_BYPASS
Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

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

ACTIVITY COEF. FLAG PITZACT
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

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

Character Flags:  J.C. nMOLES     nEXACT
Character Flags:  I.C. nMOLES     nEXACT
TEMP is an unused local variable    180000.100000000

TITRATION option requires delta(x)=0.01 meters
  Defining delta(x) as such

DIFFUS  Parameter UNUSED= nDIFFUS
CONVEC  Parameter UNUSED= CONVEC
SSDIFF  Parameter UNUSED= nSSDIFF
RESTART Parameter Value Read = nRESTART
UNUSED Parameters nPUSHPULL nMULTINJ
UNUSED parameter FRAC_FLO

TITRATION Problem:
 -) Assigning all delta(y) to 0.1 m
 -) Setting # of nodes in Y-direction to 3
 -) Setting NONREACTIVE Porosity to 0.0

Char Flags UNUSED UNUSED RHSFDIF    LHSFDIF
Char Flags UNUSED UNUSED nMOLES     nEXACT

TEMP is an unused local variable   9.9999999999999999E-021
Character Flags:  VPOROS FRFLASH VPOROS     FRFLASH

Specifying VARIABLE POROSITY for TITRATION Problem

Character Flags:  VAR_AQ_RHO VAR_AQ_RHO FRFLASH

Aqueous Density is a Function of Composition
```

Appendix B: Sample Screen Display of Np_NaCl_BM_LOG

```
Char Flag is UNUSED:  NO X DIFF nNO X DIFF
Char Flag is UNUSED:  UNIFORM UNIFORM              0

MINERAL DENSITIES, KG/M^3, IN FILE 'RHOMIN'

pmH = -log[m(H+)]                  =      11.6199
pH = -log[a(H+)]    =      11.7497
pmH = -log[m(H+)]                  =       5.9141
pH = -log[a(H+)]    =       5.3205
TITRATION Character Flags
  cdum1= TITRATE      cdum2= LOG10
  First Volume Added =          0.10 mL
  Final Volume Added =         10.00 mL

pmH = -log[m(H+)]                  =       5.9141
pH = -log[a(H+)]    =       5.3205
pmH = -log[m(H+)]                  =       6.2386
pH = -log[a(H+)]    =       5.6451
pmH = -log[m(H+)]                  =       6.5870
pH = -log[a(H+)]    =       5.9936
pmH = -log[m(H+)]                  =       8.5360
pH = -log[a(H+)]    =       7.9427
pmH = -log[m(H+)]                  =       9.4653
pH = -log[a(H+)]    =       8.8722
pmH = -log[m(H+)]                  =       9.8154
pH = -log[a(H+)]    =       9.2225
pmH = -log[m(H+)]                  =      10.0620
pH = -log[a(H+)]    =       9.4695
pmH = -log[m(H+)]                  =      10.2640
pH = -log[a(H+)]    =       9.6719
pmH = -log[m(H+)]                  =      10.4406
pH = -log[a(H+)]    =       9.8493
pmH = -log[m(H+)]                  =      10.6002
pH = -log[a(H+)]    =      10.0098
pmH = -log[m(H+)]                  =      10.7468
pH = -log[a(H+)]    =      10.1578
pmH = -log[m(H+)]                  =      10.8825
pH = -log[a(H+)]    =      10.2955
pmH = -log[m(H+)]                  =      11.0086
pH = -log[a(H+)]    =      10.4243
pmH = -log[m(H+)]                  =      11.1257
pH = -log[a(H+)]    =      10.5454
pmH = -log[m(H+)]                  =      11.2341
pH = -log[a(H+)]    =      10.6594
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 3 for explanation of this screen display.

```
Enter chemdat file name to search on: np_am
Enter rxnmin file name to search on: np_am
Enter input file name (without extension): np_nacl_bm_lin
%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_BMW_NP_AM.CHEMDAT "Initial load"
FMT_BMW_NP_AM_P90.CHEMDAT "Initial load"
Select CHEMDAT name from list above: FMT_BMW_NP_AM.CHEMDAT
Your CMS library list consists of:
    WP$NONPA_CMSROOT:[FMT]

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

Elements in CMS Library WP$NONPA_CMSROOT:[FMT]

FMT_BMW_NP_AM.RXNMIN "Initial load"
Select RXNMIN name from list above: FMT_BMW_NP_AM.RXNMIN
Your CMS library list consists of:
    WP$NONPA_CMSROOT:[FMT]

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

                    image name: "FMT_FMTIPS"
                    image file identification: "PROD PA3"
                    image file build identification: ""
                    link date/time: 21-DEC-1995 11:35:08.36
                    linker identification: "A11-14"

Entering Subroutine READDAT
reading chemical species data from CHEMDAT file
DO_BYPASS flag set to NDO_BYPASS
Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.0
DATABASE:   HSN64/FN06: Np(V)-Na-H2O-OH-Cl-CO3 (NP94);
95.01 31    Am(III)-Na-Cl-CO3-SO4-PO4 :FEAR99,PRF90,P91,RFPP90,FEP94,RXFF94:

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

ACTIVITY COEF  FLAG PITZACT
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

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

Character Flags:  J.C. nMOLES     nEXACT
Character Flags:  I.C  nMOLES     nEXACT
TEMP is an unused local variable    100000.1000000000

TITRATION option requires delta(x)=0.01 meters
   Defining delta(x) as such

DIFFUS   Parameter UNUSED= nDIFFUS
CONVECT  Parameter UNUSED= CONVECT
ISDIFF   Parameter UNUSED= nISDIFF
RESTART Parameter Value Read = nRESTART
UNUSED Parameters nITERATE nMULTIRO
UNUSED parameter FRAC FLO

TITRATION Problem:
 -> Assigning all delta(y) to 0.1 m
 -> Setting # of nodes in Y-direction to 1
 -> Setting NONREACTIVE Porosity to 0.0

Char Flags UNUSED UNUSED RECFDIFF    LRCFDIFF
```

Appendix C Sample Screen Display of Np_NaCl_BM_LIN

```
Char Flags UNUSED UNUSED [illegible]      [illegible]

TEMP is an unused local variable   9.99999999[illegible]E-021
Character Flags: VPOROS PFFLASH VPOROS     PFFLASH

Specifying VARIABLE POROSITY for TITRATION Problem

Character Flags: VAR_AQ_RHO VAR_AQ_RHO PFFLASH

Aqueous Density is a Function of Composition

Char Flag is UNUSED: NO K DIFF NO K DIFF
Char Flag is UNUSED: UNIFORM UNIFORM                0

MINERAL DENSITIES, KG/M^3, IN FILE "[illegible]"

pmH = -log[m(H+)]                    =      11.6[illegible]
pH = -log[a(H+)]       =      11.7497
pmH = -log[m(H+)]                    =      5.9141
pH = -log[a(H+)]       =      5.3205
TITRATION Character Flags
  cdum1= TITRATE      cdum2= LINEAR
  First Volume Added =          0.10 mL
  Final Volume Added =          1.40 mL

pmH = -log[m(H+)]                    =      5.9141
pH = -log[a(H+)]       =      5.3205
pmH = -log[m(H+)]                    =      6.2386
pH = -log[a(H+)]       =      5.6451
pmH = -log[m(H+)]                    =      8.4116
pH = -log[a(H+)]       =      7.8183
pmH = -log[m(H+)]                    =      9.5098
pH = -log[a(H+)]       =      8.9167
pmH = -log[m(H+)]                    =      9.7906
pH = -log[a(H+)]       =      9.1977
pmH = -log[m(H+)]                    =      9.9569
pH = -log[a(H+)]       =      9.3641
pmH = -log[m(H+)]                    =     10.0747
pH = -log[a(H+)]       =      9.4821
pmH = -log[m(H+)]                    =     10.1656
pH = -log[a(H+)]       =      9.5733
pmH = -log[m(H+)]                    =     10.2395
pH = -log[a(H+)]       =      9.6473
pmH = -log[m(H+)]                    =     10.3015
pH = -log[a(H+)]       =      9.7095
pmH = -log[m(H+)]                    =     10.3548
pH = -log[a(H+)]       =      9.7631
pmH = -log[m(H+)]                    =     10.4016
pH = -log[a(H+)]       =      9.8100
pmH = -log[m(H+)]                    =     10.4431
pH = -log[a(H+)]       =      9.8517
pmH = -log[m(H+)]                    =     10.4804
pH = -log[a(H+)]       =      9.8892
pmH = -log[m(H+)]                    =     10.5142
pH = -log[a(H+)]       =      9.9232
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 3 for explanation of this screen display.

```
Enter chemdat file name to search on: np_am
Enter chemin file name to search on: np_am
Enter input file name (without extension): np_nacl_bm
%CMS-I-LIBIS, library is NPSNONPA_CMSROOT:[FMT]
%CMS-S-LIBSET, library set
-CMS-I-SUPERSEDE, library list superseded

Elements in CMS Library NPSNONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.CHEMDAT "Initial load"
FMT_HMW_NP_AM_F60.CHEMDAT "Initial load"
Select CHEMDAT name from list above: FMT_HMW_NP_AM.CHEMDAT
Your CMS library list consists of:
    NPSNONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element NPSNONPA_CMSROOT:[FMT]FMT_HMW_NP_AM.CHEMDAT fetched

Elements in CMS Library NPSNONPA_CMSROOT:[FMT]

FMT_HMW_NP_AM.CHEMIN "Initial load"
Select CHEMIN name from list above: FMT_HMW_NP_AM.CHEMIN
Your CMS library list consists of:
    NPSNONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element NPSNONPA_CMSROOT:[FMT]FMT_HMW_NP_AM.CHEMIN fetched

                    image name: "FMT_PRP100"
                    image file identification: "PROD PA9"
                    image file build identification: ""
                    link date/time: 21-DEC-1995 11:36:38.36
                    linker identification: "A11-14"

Entering Subroutine READDAT
reading chemical species data from CHEMDAT file
DG_BYPASS flag set to NDG_BYPASS
Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl              FMT V2.0
DATABASE:   HMW94/FMT96: Np(V)-Na-K-H-Cl-ClO4 (NR94);
95.01.31    Am(III)-Na-Cl-CO3-SO4-PO4 (FESR95,FRF95,PRL,RPFT95,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
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

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

Character Flags:  O.C. nMOLES      nEXACT
Character Flags.  I.C. aMOLES      nEXACT
TEMP is an unused local variable     130000.100000000

TITRATION option requires delta(x)=0.01 meters
  Defining delta(x) as such

DIFFUS  Parameter UNUSED= nDIFFUS
CONVEC  Parameter UNUSED= CONVEC
FSDIFF  Parameter UNUSED= nOSDIFF
RESTART Parameter Value Used = nRESTART
UNUSED Parameters nPTSPTNL aMULTIN
UNUSED parameter PRO-1 FLO

TITRATION Problem:
 -: Assigning all delta(y) to 0.1 m
 -: Setting # of nodes in Y-direction to 7
 -: Setting NONREACTIVE Porosity to 0.0

Char Flags, UNUSED UNUSED nOUTPUT     nOUTPUT
```

Appendix D Sample Screen Display of Np_NaCl_BM

```
Char Flags UNUSED UNUSED [illegible]      [illegible]

TEMP is an unused local variable    [illegible]
Character Flags:  VPOROS FPFLASH VPOROS      FPFLASH

Specifying VARIABLE POROSITY for TITRATION Problem

Character Flags.   VAR_AQ_RHO VAR_AQ_RHO FPFLASH

Aqueous Density is a Function of Composition

Char Flag is UNUSED:  NO X DIFF NO X DIFF
Char Flag is UNUSED:  UNIFORM UNIFORM

MINERAL DENSITIES. KG/M^3, IN FILE "[illegible]"

pmH = -log[m(H+)]                    =       11.[illegible]
pH = -log[a(H+)]      =       11.[illegible]
pmH = -log[m(H+)]                    =       5.9141
pH = -log[a(H+)]      =       5.3205
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

pmH = -log[m(H+)]                    =       5.9141
pH = -log[a(H+)]      =       5.3205
pmH = -log[m(H+)]                    =       6.2386
pH = -log[a(H+)]      =       5.6451
pmH = -log[m(H+)]                    =       6.5870
pH = -log[a(H+)]      =       5.9936
pmH = -log[m(H+)]                    =       6.8286
pH = -log[a(H+)]      =       6.2353
pmH = -log[m(H+)]                    =       7.2930
pH = -log[a(H+)]      =       6.6996
pmH = -log[m(H+)]                    =       8.5359
pH = -log[a(H+)]      =       7.9427
pmH = -log[m(H+)]                    =       8.9250
pH = -log[a(H+)]      =       8.3317
pmH = -log[m(H+)]                    =       9.1587
pH = -log[a(H+)]      =       8.5655
pmH = -log[m(H+)]                    =       9.3098
pH = -log[a(H+)]      =       8.7166
pmH = -log[m(H+)]                    =       9.4653
pH = -log[a(H+)]      =       8.8722
pmH = -log[m(H+)]                    =       9.8154
pH = -log[a(H+)]      =       9.2225
pmH = -log[m(H+)]                    =      10.0620
pH = -log[a(H+)]      =       9.4695
pmH = -log[m(H+)]                    =      10.4406
pH = -log[a(H+)]      =       9.8493
pmH = -log[m(H+)]                    =      10.8825
pH = -log[a(H+)]      =      10.2955
pmH = -log[m(H+)]                    =      11.2341
pH = -log[a(H+)]      =      10.6594
End of AutoTitration Problem
```

Appendix E: Sample Input File "BATCH_DOC.IN"

See Table 4 for explanation of this listing.

```
'[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs'
'CHEMFILE'

'BATCH', 'UNUSED'

'nMOLES', 'nEXACT',
  1.10222364E+02   Hydrogen
  5.51654821E+01   Oxygen
  2.00000000E-01   Sodium
  1.00000000E-02   Potassium
  1.00000000E-03   Magnesium
  1.00000000E-04   Calcium
  1.10000000E-01   Chlorine
  1.00000000E-03   Sulfur
  1.00000000E-04   Carbon
  0.00000000E+00   PosIon
  0.00000000E+00   NegIon
  0.00000000E+00   Air
  1.00000000E-07   Boron
  0.00000000E+00   Bromine
  0.00000000E+00   TracerEl
  0.00000000E+00   Th(IV)
  0.00000000E+00   Am(III)
  0.00000000E+00   U(VI)
  0.00000000E+00   Np(V)
  0.00000000E+00   ClO4-(EL)
  0.00000000E+00   Phosphorus
  0.00000000E+00   Electron
  4.90605392E-17   Charge
```

Appendix F: Sample Input File "Np_NaCl_BM_LOG.IN"

See Table 5 for explanation of this listing.

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

'TITRATE', 'EXPLICIT',

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

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

```
  0.00000000E+00   Electron
 -2.37316632E-15  Charge

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

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

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

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

Appendix G: Sample Input File "Np_NaCl_BM_LIN.IN"

Note

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

See Table 5 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
```

Appendix G: Sample Input File "NP_NaCl_BM_LIN.IN"

```
   0.00000000E+00   Bromine
   0.00000000E+00   TracerEl
   0.00000000E+00   Th(IV)
   0.00000000E+00   Am(III)
   0.00000000E+00   U(VI)
   1.00000000E+01   Np(V)
   0.00000000E+00   ClO4-(EL)
   0.00000000E+00   Phosphorus
   0.00000000E+00   Electron
  -2.37316632E-15   Charge

 15  2.25d3  0.002530  1.800001d5 'nDXVARIABLE'
'nDIFFUS',
'CONVEC',
'nSSDIFF',
'nRESTART',
'nPUSHPULL','nMULTINJ',

 20 1 20 'nLOTS' 10
'nTGRAD' 'LINEAR'
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'
 3
 0.1d0 0.2d0 0.3d0
 1.d-7 0.d0 0.1829d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'
'nMOLES' 'nEXACT' Plain old pure H2O
  1.11017364E+02   Hydrogen
  5.55086220E+01   Oxygen
  0.00000000E+00   Sodium
  0.00000000E+00   Potassium
  0.00000000E+00   Magnesium
  0.00000000E+00   Calcium
  0.00000000E+00   Chlorine
  0.00000000E+00   Sulfur
  0.00000000E+00   Carbon
  0.00000000E+00   PosIon
  0.00000000E+00   NegIon
  0.00000000E+00   Air
  0.00000000E+00   Boron
  0.00000000E+00   Bromine
  0.00000000E+00   TracerEl
  0.00000000E+00   Pu(III)
  0.00000000E+00   Am(III)
  0.00000000E+00   U(VI)
  0.00000000E+00   Np(V)
  0.00000000E+00   ClO4-(EL)
  0.00000000E+00   Phosphorus
  0.00000000E+00   Electron
  0.00000000E+00   Charge

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

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

Appendix H: Sample Input File "Np_NaCl_BM.IN"

Note

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

See Table 5 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',
6
8  '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
```

Appendix H: Sample Input File "Np_NaCl_BM.IN"

```
   0.00000000E+00   Bromine
   0.00000000E+00   TracerEl
   0.00000000E+00   Th(IV)
   0.00000000E+00   Am(III)
   0.00000000E+00   U(VI)
   1.00000000E+01   Np(V)
   0.00000000E+00   ClO4-(EL)
   0.00000000E+00   Phosphorus
   0.00000000E+00   Electron
  -2.37316633E-15   Charge

 15  2.25d3  0.002530  1.800001d5 'nDXVARIABLE'
'nDIFFUS',
'CONVEC',
'nSSDIFF',
'nRESTART',
'nPUSHPULL','nMULTINJ',

 20 1 20 'nLOTS' 10
'nTGRAD' 'LINEAR'
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'
 3
 0.1d0 0.2d0 0.3d0
 1.d-7 0.d0 0.1829180 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'
'nMOLES' 'nEXACT' Plain old pure H2O
  1.11017364E+02   Hydrogen
  5.55086220E+01   Oxygen
  0.00000000E+00   Sodium
  0.00000000E+00   Potassium
  0.00000000E+00   Magnesium
  0.00000000E+00   Calcium
  0.00000000E+00   Chlorine
  0.00000000E+00   Sulfur
  0.00000000E+00   Carbon
  0.00000000E+00   PosIon
  0.00000000E+00   NegIon
  0.00000000E+00   Air
  0.00000000E+00   Boron
  0.00000000E+00   Bromine
  0.00000000E+00   TracerEl
  0.00000000E+00   Pu(III)
  0.00000000E+00   Am(III)
  0.00000000E+00   U(VI)
  0.00000000E+00   Np(V)
  0.00000000E+00   ClO4-(EL)
  0.00000000E+00   Phosphorus
  0.00000000E+00   Electron
  0.00000000E+00   Charge

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

'TITRATE','ASREAD',0.1d0,10.d0,'nINJSOLIDS'
 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
112   1.1938
113   3.4551
114   10.000
```

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

I.1 Listing

See Table 23 for explanation of this listing.

```
'DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);'
'95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)'

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

'Hydrogen' 'Oxygen' 'Sodium' 'Potassium' 'Magnesium' 'Calcium' 'Chlorine' 'Sulfur' 'Carbon' 'PosIon'
   'NegIon' 'Air' 'Boron' 'Bromine' 'TracerE1' 'Th(IV)' 'Am(III)' 'U(VI)' 'Np(V)' 'ClO4-(EL)'
   'Phosphorus' 'Electron' 'Charge'
1.0079 15.9994 22.98977 39.0983 24.305 40.08 35.453 32.06 12.011 0.0 0.0
   28.84 10.81 79.904 0.0 232.0381 243.0 238.029 237.0482 99.4506 30.974 0.0 0.0

'H2O                          WATER' 2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -95.6635     HMW84
'Na+                            Na+' 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -105.651     HMW84
'K+                              K+' 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -113.957     HMW84
'Ca++                          Ca++' 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2   1 -223.30      HMW84
'Mg++                          Mg++' 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2   1 -183.468     HMW84
'MgOH+                        MgOH+' 1 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -251.94      HMW84
'H+                              H+' 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1  0.          HMW84

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

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

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

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

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

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

'Am+++                       Am+++' 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  3   1 -241.694     FRF90
'AmCO3+                     AmCO3+' 0 3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0  1   1 -472.060     FRF90
'Am(CO3)2-                Am(CO3)2-' 0 6 0 0 0 0 0 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 -1   1 -695.880     FRF90
'Am(CO3)3=-               Am(CO3)3=-' 0 9 0 0 0 0 0 0 3 0 0 0 0 0 0 0 1 0 0 0 0 0 -3   1 -915.460     FRF90
'Am(OH)2+                 Am(OH)2+' 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  1   1 -393.647     RFFR92
'Am(OH)3(aq)             Am(OH)3(aq)' 3 3 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  0   1 -462.950     RFFR92

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

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

'NpO2OH(aged)_____________NpO2OH(aged)' 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0  0   2 -454.010     N&R94
'NpO2OH(amor)_____________NpO2OH(amor)' 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0  0   2 -452.642     N&R94
'NaNpO2CO3(s)_____________NaNpO2CO3(s)' 0 5 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0  0   2 -713.707     N&R94
'Na3NpO2(CO3)2(s)_DISABLED_DISABLED' 0 8 3 0 0 0 0 0 2 0 0 0 0 0 0 0 0 1 0 0 0  0   2  999.99      arbitrary
```

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

```
'AmOHCO3(c)_____AmOHCO3(c)' 1 4 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0  0   2 -569.980     FRF90
'Am(OH)3(s)_____Am(OH)3(s)' 3 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  0   2 -492.294     FRSR89
'NaAm(CO3)2.6H2O(c)_____' 12 12 1 0 0 0 0 0 2 0 0 0 0 0 0 0 0 1 0 0 0 0 0  0   2 -1396.494    RRFF94
'AmPO4(c)_____AmPO4(c)' 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0  0   2 -709.750     RFF94

'CaSO4_____Anhydrite'  0  4 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -533.73      HMW84
'NaK3(SO4)2__Aphthitalite/Glaserite'  0  8 1 3 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1057.05     HMW84
'CaCl2.6H2O_____Antarcticite' 12  6 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -893.65      HMW84
'CaCO3_____Aragonite'  0  3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -455.17      HMW84
'K2SO4_____Arcanite'  0  4 0 2 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -532.39      HMW84
'MgCl2.6H2O_____Bischofite' 12  6 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -853.1       HMW84
'Na2Mg(SO4)2.4H2O_____Bloedite'  8 12 2 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1383.6      HMW84
'Mg(OH)2_____Brucite'  2  2 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -335.4       HMW84
'Na6CO3(SO4)2_____Burkeite'  0 11 6 0 0 0 0 2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1449.4      HMW84
'CaCO3_____Calcite'  0  3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -455.6       HMW84
'CaCl2.4H2O_____CaCl2_Tetrahydrite'  8  4 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -698.7       HMW84
'Ca4Cl2(OH)6.13H2O__CaOxychloride A' 32 19 0 0 0 4 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -2658.45     HMW84
'Ca2Cl2(OH)2.H2O___CaOxychloride B'  4  3 0 0 0 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -778.41      HMW84
'KMgCl3.6H2O_____Carnallite' 12  6 0 1 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1020.3      HMW84
'MgSO4.7H2O_____Epsomite' 14 11 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1157.83     HMW84
'CaNa2(CO3)2.5H2O_____Gaylussite' 10 11 2 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1360.5      HMW84
'Na2Ca(SO4)2_____Glauberite'  0  8 2 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1047.45     HMW84
'CaSO4.2H2O_____Gypsum'  4  6 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -725.56      HMW84
'NaCl_____Halite'  0  0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -154.99      HMW84
'MgSO4.6H2O_____Hexahydrite' 12 10 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1061.60     HMW84
'KMgClSO4.3H2O_____Kainite'  6  7 0 1 1 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -938.2       HMW84
'KHCO3_____Kalicinite'  1  3 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -350.06      HMW84
'MgSO4.H2O_____Kieserite'  2  5 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -579.80      HMW84
'K2Mg(SO4)2.4H2O_____Leonite'  8 12 0 2 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1403.97     HMW84
'Na4Ca(SO4)3.2H2O_____Labile_Salt'  4 14 4 0 0 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1751.45     HMW84
'MgCO3_____Magnesite'  0  3 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -414.45      HMW84
'Mg2Cl(OH)3.4H2O_____MgOxychloride' 11  7 0 0 2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1029.6      HMW84
'KHSO4_____Mercallite'  1  4 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -417.57      HMW84
'Na2SO4.10H2O_____Mirabilite' 20 14 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1471.15     HMW84
'K8H6(SO4)7_____Misenite'  6 28 0 8 0 0 0 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -3039.24     HMW84
'NaHCO3_____Nahcolite'  1  3 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -343.33      HMW84
'Na2CO3.10H2O_____Natron' 20 13 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1382.78     HMW84
'MgCO3.3H2O_____Nesquehonite'  6  6 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -695.3       HMW84
'K2Mg(SO4)2.6H2O Picromerite/Schoen' 12 14 0 2 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1596.1      HMW84
'Na2Ca(CO3)2.2H2O_____Pirssonite'  4  8 2 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1073.1      HMW84
'K2MgCa2(SO4)4.2H2O_____Polyhalite'  4 18 0 2 1 2 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -2282.5      HMW84
'Ca(OH)2_____Portlandite'  2  2 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -362.12      HMW84
'K2CO3.3/2H2O___Potassium_Carbonate' 3 4.5 0 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -577.37     HMW84
'K8H4(CO3)6.3H2O___K-Sequicarbonate' 10 21 0 8 0 0 0 0 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -2555.4     HMW84
'KNaCO3.6H2O_____K-Na-Carbonate' 12  9 1 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1006.8      HMW84
'K2NaH(CO3)2.2H2O___Potassium_Trona'  5  8 1 2 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -971.74      HMW84
'K3H(SO4)2__Sesquipotassium_Sulfate'  1  8 0 3 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -950.8       HMW84
'Na3H(SO4)2____Sesquisodium_Sulfate'  1  8 3 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -919.6       HMW84
'Na2CO3.7H2O____Na2CO3-Heptahydrate' 14 10 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1094.95     HMW84
'KCl_____Sylvite'  0  0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -164.84      HMW84
'K2Ca(SO4)2.H2O_____Syngenite'  2  9 0 2 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -1164.8      HMW84
'Mg2CaCl6.12H2O_____Tachyhydrite' 24 12 0 0 2 1 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -2015.9      HMW84
'Na2SO4_____Thenardite'  0  4 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -512.35      HMW84
'Na2CO3.H2O_____Thermonatrite'  2  4 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -518.8       HMW84
'Na3H(CO3)2.2H2O_____Trona'  5  8 3 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2 -960.38      HMW84
'Na2B4O7.10H2O_____Borax' 20 17 2 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0  2 -2224.16     FW86
'B(OH)3_____Borix_Acid_Solid'  3  3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  2 -390.88      FW86
'KB5O8.4H2O____K-Pentaborate_(3D_C)'  8 12 0 1 0 0 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0  2 -1770.26     FW86
'K2B4O7.4H2O___K-Tetraborate_(3D_C)'  8 11 0 2 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0  2 -1663.47     FW86
'NaBO2.4H2O_____Sodium_Metaborate'  8  6 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  2 -761.42      FW86
'NaB5O8.5H2O_____Sodium_Pentaborate' 10 13 1 0 0 0 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0  2 -1854.80     FW86
'NaBO2.NaCl.2H2O___Teepleite_(20_C)'  4  4 2 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  2 -725.77      FW86

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

  1  .0765     .2644     .0      .00127   Na+ Cl-            HMW84 (beta0, beta1, beta2, cphi)
  1  .01958   1.113      .0      .00497   Na+ SO4=           HMW84
  1  .0454     .398      .0      .0       Na+ HSO4-          HMW84
  1  .0864     .253      .0      .0044    Na+ OH-            HMW84
  1  .0277     .0411     .0      .0       Na+ HCO3-          HMW84
  1  .0399    1.389      .0      .0044    Na+ CO3=           HM284
  1 -.0427     .089      .0      .0114    Na+ B(OH)4-        FW86
  1 -.056     -.910      .0      .0       Na+ B3O3(OH)4-     FW86
  1 -.11      -.40       .0      .0       Na+ B4O5(OH)4=     FW86
  1  .0        .0        .0      .0       Na+ Br-
  1  .0      -8.37       .0      .0       Na+ Am(CO3)2-      RRFF94
  1 -.94      8.1        .0      .418     Na+ Am(CO3)3=-     RRFF94,FRF90
  1  .0554     .2755     .0     -.00118   Na+ ClO4-          P91
  1  .0        .0        .0      .0       Na+ NpO2(OH)2-     NR94
  1  .161      .0        .0      .0       Na+ NpO2CO3-       NR94
  1  .407      .0        .0      .0       Na+ NpO2(CO3)2=-   NR94
  1  1.97     16.        .0      .0       Na+ NpO2(CO3)3==-  NR94
  1 -.0533     .0396     .0      .00795   Na+ H2PO4-         P91
  1 -.0583    1.466      .0      .0294    Na+ HPO4=          P91
  1  .1781    3.851      .0     -.05154   Na+ PO4=-          P91
```

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

```
 1  .04835    .2122     .0     -.00084   K+ Cl-              HMW84
 1  .04995    .7793     .0      .0       K+ SO4=             HMW84
 1 -.0003     .1735     .0      .0       K+ HSO4-            HMW84
 1  .1298     .320      .0      .0041    K+ OH-              HMW84
 1  .0296    -.013      .0     -.008     K+ HCO3-            HMW84
 1  .1488    1.43       .0     -.0015    K+ CO3=             HMW84
 1  .035      .14       .0      .0       K+ B(OH)4-          FW86
 1 -.13       .0        .0      .0       K+ B3O3(OH)4-       FW86
 1 -.022      .0        .0      .0       K+ B4O5(OH)4=       FW86
 1  .0        .0        .0      .0       K+ Br-
 1  .0        .0        .0      .0       K+ Am(CO3)2-
 1  .0        .0        .0      .0       K+ Am(CO3)3=-
 1  .0        .0        .0      .0       K+ ClO4-
 1  .0        .0        .0      .0       K+ NpO2(OH)2-
 1  .0        .0        .0      .0       K+ NpO2CO3-
 1  .0        .0        .0      .0       K+ NpO2(CO3)2=-
 1  .0        .0        .0      .0       K+ NpO2(CO3)3==-
 1 -.0678    -.1042     .0      .0       K+ H2PO4-           P91
 1  .0248    1.274      .0      .0164    K+ HPO4=            P91
 1  .3729    3.972      .0     -.08680   K+ PO4=-            P91

 1  .3159    1.614      .0     -.00034   Ca++ Cl-            HMW84
 2  .20      3.1973   -54.24    .0       Ca++ SO4=           HMW84
 1  .2145    2.53       .0      .0       Ca++ HSO4-          HMW84
 1 -.1747    -.2303    -5.72    .0       Ca++ OH-            HMW84
 1  .4        2.977     .0      .0       Ca++ HCO3-          HMW84
 2  .0        .0        .0      .0       Ca++ CO3=           HMW84
 1  .0        .0        .0      .0       Ca++ B(OH)4-        FW86
 1  .0        .0        .0      .0       Ca++ B3O3(OH)4-     FW86
 1  .0        .0        .0      .0       Ca++ B4O5(OH)4=     FW86
 1  .0        .0        .0      .0       Ca++ Br-
 1  .0        .0        .0      .0       Ca++ Am(CO3)2-
 3  .0        .0        .0      .0       Ca++ Am(CO3)3=-
 1  .4511    1.756      .0     -.00500   Ca++ ClO4-          P91
 1  .0        .0        .0      .0       Ca++ NpO2(OH)2-
 1  .0        .0        .0      .0       Ca++ NpO2CO3-
 3  .0        .0        .0      .0       Ca++ NpO2(CO3)2=-
 3  .0        .0        .0      .0       Ca++ NpO2(CO3)3==-
 1  .0        .0        .0      .0       Ca++ H2PO4-
 2  .0        .0        .0      .0       Ca++ HPO4=
 3  .0        .0        .0      .0       Ca++ PO4=-

 1  .35235   1.6815     .0      .00519   Mg++ Cl-            HMW84
 2  .2210    3.343    -37.23    .025     Mg++ SO4=           HMW84
 1  .4746    1.729      .0      .0       Mg++ HSO4-          HMW84
 1  .0        .0        .0      .0       Mg++ OH-            HMW84
 1  .329      .6072     .0      .0       Mg++ HCO3-          HMW84
 2  .0        .0        .0      .0       Mg++ CO3=           HMW84
 1  .0        .0        .0      .0       Mg++ B(OH)4-        FW86
 1  .0        .0        .0      .0       Mg++ B3O3(OH)4-     FW86
 1  .0        .0        .0      .0       Mg++ B4O5(OH)4=     FW86
 1  .0        .0        .0      .0       Mg++ Br-
 1  .0        .0        .0      .0       Mg++ Am(CO3)2-
 3  .0        .0        .0      .0       Mg++ Am(CO3)3=-
 1  .4961    2.008      .0      .009578  Mg++ ClO4-          P91
 1  .0        .0        .0      .0       Mg++ NpO2(OH)2-
 1  .0        .0        .0      .0       Mg++ NpO2CO3-
 3  .0        .0        .0      .0       Mg++ NpO2(CO3)2=-
 3  .0        .0        .0      .0       Mg++ NpO2(CO3)3==-
 1  .0        .0        .0      .0       Mg++ H2PO4-
 2  .0        .0        .0      .0       Mg++ HPO4=
 3  .0        .0        .0      .0       Mg++ PO4=-

 1 -.10      1.658      .0      .0       MgOH+ Cl-           HMW84
 1  .0        .0        .0      .0       MgOH+ SO4=          HMW84
 1  .0        .0        .0      .0       MgOH+ HSO4-         HMW84
 1  .0        .0        .0      .0       MgOH+ OH-           HMW84
 1  .0        .0        .0      .0       MgOH+ HCO3-         HMW84
 1  .0        .0        .0      .0       MgOH+ CO3=          HMW84
 1  .0        .0        .0      .0       MgOH+ B(OH)4-
 1  .0        .0        .0      .0       MgOH+ B3O3(OH)4-
 1  .0        .0        .0      .0       MgOH+ B4O5(OH)4=
 1  .0        .0        .0      .0       MgOH+ Br-
 1  .0        .0        .0      .0       MgOH+ Am(CO3)2-
 1  .0        .0        .0      .0       MgOH+ Am(CO3)3=-
 1  .0        .0        .0      .0       MgOH+ ClO4-
 1  .0        .0        .0      .0       MgOH+ NpO2(OH)2-
 1  .0        .0        .0      .0       MgOH+ NpO2CO3-
 1  .0        .0        .0      .0       MgOH+ NpO2(CO3)2=-
 1  .0        .0        .0      .0       MgOH+ NpO2(CO3)3==-
 1  .0        .0        .0      .0       MgOH+ H2PO4-
 1  .0        .0        .0      .0       MgOH+ HPO4=
 1  .0        .0        .0      .0       MgOH+ PO4=-

 1  .1775    .2945      .0      .0008    H+ Cl-              HMW84
 1  .0298     .0        .0      .0438    H+ SO4=             HMW84
 1  .2065    .5556      .0      .0       H+ HSO4-            HMW84
 1  .0        .0        .0      .0       H+ OH-              HMW84
 1  .0        .0        .0      .0       H+ HCO3-            HMW84
 1  .0        .0        .0      .0       H+ CO3=             HMW84
```

```
1 .0       .0      .0      .0       H+ B(OH)4-          FW86
1 .0       .0      .0      .0       H+ B3O3(OH)4-       FW86
1 .0       .0      .0      .0       H+ B4O5(OH)4=       FW86
1 .0       .0      .0      .0       H+ Br-
1 .0       .0      .0      .0       H+ Am(CO3)2-
1 .0       .0      .0      .0       H+ Am(CO3)3=-
1 .1747    .2931   .0      .00819   H+ ClO4-            P91
1 .0       .0      .0      .0       H+ NpO2(OH)2-
1 .0       .0      .0      .0       H+ NpO2CO3-
1 .0       .0      .0      .0       H+ NpO2(CO3)2=-
1 .0       .0      .0      .0       H+ NpO2(CO3)3==-
1 .0       .0      .0      .0       H+ H2PO4-
1 .0       .0      .0      .0       H+ HPO4=
1 .0       .0      .0      .0       H+ PO4=-

1 .16      .0      .0      .0       MgB(OH)4+ Cl-       HMW84
1 .0       .0      .0      .0       MgB(OH)4+ SO4=      HMW84
1 .0       .0      .0      .0       MgB(OH)4+ HSO4-     HMW84
1 .0       .0      .0      .0       MgB(OH)4+ OH-       HMW84
1 .0       .0      .0      .0       MgB(OH)4+ HCO3-     HMW84
1 .0       .0      .0      .0       MgB(OH)4+ CO3=      HMW84
1 .0       .0      .0      .0       MgB(OH)4+ B(OH)4-
1 .0       .0      .0      .0       MgB(OH)4+ B3O3(OH)4-
1 .0       .0      .0      .0       MgB(OH)4+ B4O5(OH)4=
1 .0       .0      .0      .0       MgB(OH)4+ Br-
1 .0       .0      .0      .0       MgB(OH)4+ Am(CO3)2-
1 .0       .0      .0      .0       MgB(OH)4+ Am(CO3)3=-
1 .0       .0      .0      .0       MgB(OH)4+ ClO4-
1 .0       .0      .0      .0       MgB(OH)4+ NpO2(OH)2-
1 .0       .0      .0      .0       MgB(OH)4+ NpO2CO3-
1 .0       .0      .0      .0       MgB(OH)4+ NpO2(CO3)2=-
1 .0       .0      .0      .0       MgB(OH)4+ NpO2(CO3)3==-
1 .0       .0      .0      .0       MgB(OH)4+ H2PO4-
1 .0       .0      .0      .0       MgB(OH)4+ HPO4=
1 .0       .0      .0      .0       MgB(OH)4+ PO4=-

1 .12      .0      .0      .0       CaB(OH)4+ Cl-
1 .0       .0      .0      .0       CaB(OH)4+ SO4=      HMW84
1 .0       .0      .0      .0       CaB(OH)4+ HSO4-     HMW84
1 .0       .0      .0      .0       CaB(OH)4+ OH-       HMW84
1 .0       .0      .0      .0       CaB(OH)4+ HCO3-     HMW84
1 .0       .0      .0      .0       CaB(OH)4+ CO3=      HMW84
1 .0       .0      .0      .0       CaB(OH)4+ B(OH)4-
1 .0       .0      .0      .0       CaB(OH)4+ B3O3(OH)4-
1 .0       .0      .0      .0       CaB(OH)4+ B4O5(OH)4=
1 .0       .0      .0      .0       CaB(OH)4+ Br-
1 .0       .0      .0      .0       CaB(OH)4+ Am(CO3)2-
1 .0       .0      .0      .0       CaB(OH)4+ Am(CO3)3=-
1 .0       .0      .0      .0       CaB(OH)4+ ClO4-
1 .0       .0      .0      .0       CaB(OH)4+ NpO2(OH)2-
1 .0       .0      .0      .0       CaB(OH)4+ NpO2CO3-
1 .0       .0      .0      .0       CaB(OH)4+ NpO2(CO3)2=-
1 .0       .0      .0      .0       CaB(OH)4+ NpO2(CO3)3==-
1 .0       .0      .0      .0       CaB(OH)4+ H2PO4-
1 .0       .0      .0      .0       CaB(OH)4+ HPO4=
1 .0       .0      .0      .0       CaB(OH)4+ PO4=-

1 .6117    5.403   .0      -0.0284  Am+++ Cl-           FRSR89
3 3.0398   .0      -2500   .0       Am+++ SO4=          RFF94
1 .0       .0      .0      .0       Am+++ HSO4-
1 .0       .0      .0      .0       Am+++ OH-
1 .0       .0      .0      .0       Am+++ HCO3-
3 .0       .0      .0      .0       Am+++ CO3=
1 .0       .0      .0      .0       Am+++ B(OH)4-
1 .0       .0      .0      .0       Am+++ B3O3(OH)4-
1 .0       .0      .0      .0       Am+++ B4O5(OH)4=
1 .0       .0      .0      .0       Am+++ Br-
1 .0       .0      .0      .0       Am+++ Am(CO3)2-
3 .0       .0      .0      .0       Am+++ Am(CO3)3=-
1 .80      5.35    .0      -0.0048  Am+++ ClO4-         FRF90
1 .0       .0      .0      .0       Am+++ NpO2(OH)2-
1 .0       .0      .0      .0       Am+++ NpO2CO3-
3 .0       .0      .0      .0       Am+++ NpO2(CO3)2=-
3 .0       .0      .0      .0       Am+++ NpO2(CO3)3==-
1 .0       .0      -92.9   .0       Am+++ H2PO4-        RFF94
3 .0       .0      .0      .0       Am+++ HPO4=
3 .0       .0      .0      .0       Am+++ PO4=-

1 .0       .0      .0      .0       AmCO3+ Cl-
1 .0       .0      .0      .0       AmCO3+ SO4=
1 .0       .0      .0      .0       AmCO3+ HSO4-
1 .0       .0      .0      .0       AmCO3+ OH-
1 .0       .0      .0      .0       AmCO3+ HCO3-
1 .0       .0      .0      .0       AmCO3+ CO3=
1 .0       .0      .0      .0       AmCO3+ B(OH)4-
1 .0       .0      .0      .0       AmCO3+ B3O3(OH)4-
1 .0       .0      .0      .0       AmCO3+ B4O5(OH)4=
1 .0       .0      .0      .0       AmCO3+ Br-
1 .0       .0      .0      .0       AmCO3+ Am(CO3)2-
1 .0       .0      .0      .0       AmCO3+ Am(CO3)3=-
```

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

```
 1  .0        .0        .0      .0       AmCO3+ ClO4-
 1  .0        .0        .0      .0       AmCO3+ NpO2(OH)2-
 1  .0        .0        .0      .0       AmCO3+ NpO2CO3-
 1  .0        .0        .0      .0       AmCO3+ NpO2(CO3)2=-
 1  .0        .0        .0      .0       AmCO3+ NpO2(CO3)3==-
 1  .0        .0        .0      .0       AmCO3+ H2PO4-
 1  .0        .0        .0      .0       AmCO3+ HPO4=
 1  .0        .0        .0      .0       AmCO3+ PO4=-

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

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

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


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


 .02  -.006  -.050  .03  -.02  -.065 .12 .074 0. 0. 0. 0. 0. 0. 0. 0. .1  0. 0. Cl:          (anions  2-20)
 0.   -.013  .01   .02   -.012  .10  .12  0.  0. 0. 0. 0. 0. 0. 0. 0. 0.  0.    SO4:         (anions  3-20)
 0.    0.     0.    0.   0.     0.   0.   0.  0. 0. 0. 0. 0. 0. 0. 0. 0.        HSO4:        (anions  4-20)
```

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

```
 0.    .10    0.    0.    0.      0.    0.    0.  0. 0. 0. 0. 0. 0. 0. 0.        OH:          (anions  5-20)
-.04   0.     -.10  -.087 0.      0.    0.    0.  0. 0. 0. 0. 0. 0. 0.          HCO3:        (anions  6-20)
 0.    0.     0.    0.    0.      0.    0.    0.  0. 0. 0. 0. 0. 0.              CO3:         (anions  7-20)
 0.    0.     0.    0.    0.      0.    0.    0.  0. 0. 0. 0. 0. 0.              B(OH)4:      (anions  8-20)
 0.    0.     0.    0.    0.      0.    0.    0.  0. 0. 0. 0. 0.                 B3O3(OH)4:   (anions  9-20)
 0.    0.     0.    0.    0.      0.    0.    0.  0. 0. 0.                       B4O5(OH)4:   (anions 10-20)
 0.    0.     0.    0.    0.      0.    0.    0.  0. 0.                          Br:          (anions 11-20)
 0.    0.     0.    0.    0.      0.    0.    0.  0.                            Am(CO3)2-:   (anions 12-20)
 0.    0.     0.    0.    0.      0.    0.    0.                                Am(CO3)3=-:  (anions 13-20)
 0.    0.     0.    0.    0.      0.    0.                                      ClO4-:       (anions 14-20)
 0.    0.     0.    0.    0.      0.                                            NpO2(OH)2-:  (anions 15-20)
 0.    0.     0.    0.    0.                                                    NpO2CO3-:    (anions 16-20)
 0.    0.     0.    0.                                                          NpO2(CO3)2=-:(anions 17-20)
 0.    0.     0.                                                                NPC3==-:     (anions 18-20)
 0.    0.                                                                       H2PO4-:      (anions 19-20)
 0.                                                                             HPO4=:       (anions 20-20)

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

 -.025    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -Ca:
 -.022  -.048    .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -Mg:
    .0    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -MgOH:
 -.011   .197 -.0265  .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -H :
    .0    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -MgB(OH)4+
    .0    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -CaB(OH)4+
    .0    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -Am+++
    .0    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -AmCO3+
    .0    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -Th++++
    .0    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -UO2++
    .0    .0     .0   .0  .0   .0  .0  .0   .0   .0  .0  .0  .0   .0 0 0 0 0 0 0  K -NpO2++

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

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

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

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

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

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

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

```
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0  CaB(OH)4-UO2++
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0 0 0 0 0 0 0 0  CaB(OH)4-NpO2++

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

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

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

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

 .0014     .0 -.018 -.004 .0    .0 .0 .0    .0   .0   .0   .0   .0  Cl-SO4:(Na,K,Ca,Mg,
 -.006     .0    .0    .0 .0 .013 .0 .0    .0   .0   .0   .0   .0  Cl-HSO4:   MgOH,H,MgB(OH)3,
 -.006 -.006 -.025    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-OH:     CaB(OH)4,Am+++,
 -.015     .0    .0 -.096 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-HCO3:   AmCO3+,Th++++,
  .0085  .004    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-CO3:    UO2++,NpO2+)
-.0073     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-B(OH)4:
 -.024     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-B3O3(OH)4:
  .026     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-B4O5(OH)4:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-Br:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-Am(CO3)2:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-Am(CO3)3:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-ClO4-:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-NpO2(OH)2-:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-NpO2CO3-:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-NpO2(CO3)2=-:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-NpO2(CO3)3==-:
    .0   -.01    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-H2PO4-:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-HPO4=:
    .0     .0    .0    .0 .0   .0 .0 .0    .0   .0   .0   .0   .0  Cl-PO4=-:

-.0094 -.0677 .0 -.0425 .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-HSO4:
 -.009 -.050 .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-OH:
 -.005 .0    .0   -.161 .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-HCO3:
 -.005 -.009 .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-CO3:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-B(OH)4:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-B3O3(OH)4:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-B4O5(OH)4:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-Br:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-Am(CO3)2:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-Am(CO3)3:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-ClO4-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-NpO2(OH)2-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-NpO2CO3-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-NpO2(CO3)2=-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-NpO2(CO3)3=*-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-H2PO4-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-HPO4=:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  SO4-PO4=-:

 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-OH:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-HCO3-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-CO3=:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-B(OH)4-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-B3O3(OH)4:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-B4O5(OH)4:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-Br-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-Am(CO3)2-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-Am(CO3)2=-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-ClO4-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-NpO2(OH)2-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-NpO2CO3-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-NpO2(CO3)2=-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-NpO2(CO3)3==-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-H2PO4-:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-HPO4=:
 .0     .0   .0    .0   .0 .0   .0    .0   .0   .0   .0   .0   .0  HSO4-PO4=-:

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

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

```
619
620  .002 .012  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-CO3:
621  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-B(OH)4:
622  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-B3O3(OH)4:
623  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-B4O5(OH)4:
624  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-Br:
625  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-Am(CO3)2:
626  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-Am(CO3)3:
627  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-ClO4-:
628  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-NpO2(OH)2-:
629  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-NpO2CO3-:
630  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-NpO2(CO3)2=-:
631  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-NpO2(CO3)3==-:
632  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-H2PO4-:
633  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-HPO4=:
634  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  HCO3-PO4=-:
635
636  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-B(OH)4-:
637  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-B3O3(OH)4:
638  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-B4O5(OH)4:
639  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-Br:
640  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-Am(CO3)2:
641  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-Am(CO3)3:
642  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-ClO4-:
643  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-NpO2(OH)2-:
644  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-NpO2CO3-:
645  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-NpO2(CO3)2=-:
646  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-NpO2(CO3)3==-:
647  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-H2PO4-:
648  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-HPO4=:
649  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  CO3-PO4=-:
650
651  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-B3O3(OH)4:
652  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-B4O5(OH)4:
653  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-Br:
654  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-Am(CO3)2:
655  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-Am(CO3)3:
656  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-ClO4-:
657  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-NpO2(OH)2-:
658  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-NpO2CO3-:
659  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-NpO2(CO3)2=-:
660  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-NpO2(CO3)3==-:
661  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-H2PO4-:
662  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-HPO4=:
663  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B(OH)4-PO4=-:
664
665  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-B4O5(OH)4:
666  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-Br:
667  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-Am(CO3)2:
668  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-Am(CO3)3:
669  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-ClO4-:
670  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-NpO2(OH)2-
671  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-NpO2CO3-:
672  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-NpO2(CO3)2=-:
673  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-NpO2(CO3)3==-:
674  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-H2PO4-:
675  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-HPO4=:
676  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B3O3(OH)4-PO4=-:
677
678  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=Br:
679  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=Am(CO3)2:
680  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=Am(CO3)3:
681  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=ClO4-:
682  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=NPO2(OH)2-
683  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=NpO2CO3-:
684  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=NpO2(CO3)2=-:
685  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=NpO2(CO3)3==-:
686  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=H2PO4-:
687  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=HPO4=:
688  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  B4O5(OH)4=PO4=-:
689
690  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-Am(CO3)2:
691  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-Am(CO3)3:
692  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-ClO4-:
693  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-NpO2(OH)2-:
694  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-NpO2CO3-:
695  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-NpO2(CO3)2=-:
696  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-NpO2(CO3)3==-:
697  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-H2PO4-:
698  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-HPO4=:
699  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Br-PO4=-:
700
701  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-Am(CO3)3:
702  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-ClO4-:
703  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-NpO2(OH)2-:
704  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-NpO2CO3-:
705  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-NpO2(CO3)2=-:
706  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-NpO2(CO3)3==-:
707  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-H2PO4-:
708  .0   .0   .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  Am(CO3)2-HPO4=:
```

```
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  Am(CO3)2-PO4=-:

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

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

 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(OH)2--NpO2CO3-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(OH)2--NpO2(CO3)2=-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(OH)2--NpO2(CO3)3==-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(OH)2-H2PO4-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(OH)2-HPO4=:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(OH)2-PO4=-:

 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2CO3-NpO2(CO3)2=-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2CO3-NpO2(CO3)3==-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2CO3-H2PO4-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2CO3-HPO4=:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2CO3-PO4=-:

 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpC2-NpO2(CO3)3==-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpC2-H2PO4-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpC2-HPO4=:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpC2-PO4=-:

 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(CO3)3-H2PO4-:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(CO3)3-HPO4=:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  NpO2(CO3)3-PO4=-:

 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  H2PO4-HPO4=:
 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  H2PO4-PO4=-:

 .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   .0    .0  HPO4-PO4=-:

 .100 .051  .183 .183 .0  .0  .0  .0  .0  .0  .0  .0  .0   CO2-Cations     HMW84
   .0   .0    .0   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0   CaCO3-Cations   HMW84
   .0   .0    .0   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0   MgCO3-Cations   HMW84
-.097 -.14    .0   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0   B(OH)3-Cations  FW86
   .0   .0    .0   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0   NpO2OH-Cations
   .0 -.07    .0   .0 .0 .29  .0  .0  .0  .0  .0  .0  .0   H3PO4-Cations   PS76

-.005 .097 -.003   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0 0     0 0 0 CO2-Anions    HMW84
   .0   .0    .0   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0 0     0 0 0 CaCO3-Anions  HMW84
   .0   .0    .0   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0 0     0 0 0 MgCO3-Anions  HMW84
 .091 .018    .0   .0 .0  .0  .0 -.20 .0  .0  .0  .0  .0 0 0 0 0     0 0 0 B(OH)3-Anions FW86
   .0   .0    .0   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0 0     0 0 0 NpO2OH-Anions
   .0   .0    .0   .0 .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0 0 -.4 0 0 H3PO4-Anions  PS76

.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0   CO2-Cation-Anion
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0   (Cations down, Anions across)
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0

.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0   CaCO3-Cation-Anion
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0

.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0   MgCO3-Cation-Anion
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0   .0 0 0 0
```

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

.0      .046 .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0   B(OH)3-Cation-Anion FW86
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0   (Cations down, Anions across)
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
-.0102  .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0      .0   .0 .0 .0 .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0

.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0   NpO2OH(aq)-Cation-Anion
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0

.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0   H3PO4-Cation-Anion
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0
.0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0  .0 0 0 0

 2  3  4  5  6  7 22 21 43 44 49 50 37                   cation  mapping for ELMAP(1,)
 8  9 10 11 12 13 18 19 20 23 45 46 24 39 40 41 42 34 35 36   anion   mapping for ELMAP(2,)
14 15 16 17 38 33                                        neutral mapping for ELMAP(3,)

'nEQUALACT' 0

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



FRSR89 ==  Felmy, Rai, Schramke, and Ryan (1989) RCA 48 pp.29-35
FRF90  ==  Felmy, Rai, and Fulton (1990) RCA 50 pp.193-204
PS76   ==  Pitzer and Silvester (1976) J Soln Chem 5#4 pp.269-278
P91    ==  Pitzer (1991) CRC Handbook, Activity Coef in Electrolyte Solns
RFF92  ==  Rai, Felmy, and Fulton (1992)  RCA 56 pp.7-14
RFFR92 ==  Rai, Felmy, Fulton, and Ryan (1992) RCA 58/59 pp.9-16
RFF94  ==  Rai, Felmy, and Fulton (1994)
RRFF94 ==  Rao, Rai, Felmy, and Fulton (1994) SAND94-1948J for RCA

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

I.2 References Cited in Listing

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

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

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

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

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

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

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

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

Rai, D., A.R. Felmy, and R.W. Fulton. 1994. "The Nd^{3+} and Am^{3+} Ion Interactions with SO_4^{2-} and their Influence on NdPO4(c) Solubility." *Journal of Solution Chemistry.* submitted June 1994.

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

Rao, L., D. Rai, A.R. Felmy, and RW. Fulton. 1994. "Solubility of $NaNd(CO_3)_2 \cdot 6H_2O$ in Concentrated Sodium Carbonate and Sodium Bicarbonate Solutions." *Radiochimica Acta* vol. ___: ___-___. SAND94-1948J.

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

See Table 24 for explanation of this listing.

```
Temperature is Hard Coded as 298.15K
[.PD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs                FMT V2.0
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (MR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RPFR92,RFF94,RRFF94)

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


Species Order for Pitzer Parameters

Cations

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

Anions

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


Neutral

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

Cation-Anion Binary Interaction Parameters

Cation         Anion              Beta(0)     Beta(1)     Beta(2)     Cphi     Alpha-Values
Na+            Cl-                0.07650     0.26440     0.00000     0.00127  (2.0,12) 1-1,1-2,1-3
Na+            SO4=               0.01958     1.11300     0.00000     0.00497  (2.0,12) 1-1,1-2,1-3
Na+            HSO4-              0.04540     0.39800     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            OH-                0.08640     0.25300     0.00000     0.00440  (2.0,12) 1-1,1-2,1-3
Na+            HCO3-              0.02770     0.04110     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            CO3=               0.03990     1.38900     0.00000     0.00440  (2.0,12) 1-1,1-2,1-3
Na+            B(OH)4-           -0.04270     0.08900     0.00000     0.01140  (2.0,12) 1-1,1-2,1-3
Na+            B3O3(OH)4-        -0.05600    -0.91000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            B4O5(OH)4=        -0.11000    -0.40000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            Br-                0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            Am(CO3)2-          0.00000    -8.37000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            Am(CO3)3=-        -0.94000     8.10000     0.00000     0.41800  (2.0,12) 1-1,1-2,1-3
Na+            ClO4-              0.05540     0.27550     0.00000    -0.00118  (2.0,12) 1-1,1-2,1-3
Na+            NpO2(OH)2-         0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            NpO2CO3-           0.16100     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            NpO2(CO3)2=-       0.40700     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            NpO2(CO3)3==-      1.97000    16.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Na+            H2PO4-            -0.05330     0.03960     0.00000     0.00795  (2.0,12) 1-1,1-2,1-3
Na+            HPO4=             -0.05830     1.46600     0.00000     0.02940  (2.0,12) 1-1,1-2,1-3
Na+            PO4=-              0.17810     3.85100     0.00000    -0.05154  (2.0,12) 1-1,1-2,1-3
K+             Cl-                0.04835     0.21220     0.00000    -0.00084  (2.0,12) 1-1,1-2,1-3
K+             SO4=               0.04995     0.77930     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             HSO4-             -0.00030     0.17350     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             OH-                0.12980     0.32000     0.00000     0.00410  (2.0,12) 1-1,1-2,1-3
K+             HCO3-              0.02960    -0.01300     0.00000    -0.00800  (2.0,12) 1-1,1-2,1-3
K+             CO3=               0.14880     1.43000     0.00000    -0.00150  (2.0,12) 1-1,1-2,1-3
K+             B(OH)4-            0.03500     0.14000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             B3O3(OH)4-        -0.13000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             B4O5(OH)4=        -0.02200     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             Br-                0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             Am(CO3)2-          0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             Am(CO3)3=-         0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             ClO4-              0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             NpO2(OH)2-         0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             NpO2CO3-           0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             NpO2(CO3)2=-       0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             NpO2(CO3)3==-      0.00000     0.00000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             H2PO4-            -0.06780    -0.10420     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
K+             HPO4=              0.02480     1.27400     0.00000     0.01640  (2.0,12) 1-1,1-2,1-3
K+             PO4=-              0.37290     3.97200     0.00000    -0.08680  (2.0,12) 1-1,1-2,1-3
Ca++           Cl-                0.31590     1.61400     0.00000    -0.00034  (2.0,12) 1-1,1-2,1-3
Ca++           SO4=               0.20000     3.19730   -54.24000     0.00000  (1.4,12) 2-2
Ca++           HSO4-              0.21450     2.53000     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Ca++           OH-               -0.17470    -0.23030    -5.72000     0.00000  (2.0,12) 1-1,1-2,1-3
Ca++           HCO3-              0.40000     2.97700     0.00000     0.00000  (2.0,12) 1-1,1-2,1-3
Ca++           CO3=               0.00000     0.00000     0.00000     0.00000  (1.4,12) 2-2
```

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

83	Ca++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
84	Ca++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
85	Ca++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
86	Ca++	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
87	Ca++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
88	Ca++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
89	Ca++	*ClO4-*	*0.45110*	*1.75600*	*0.00000*	*-0.00500*	(2.0,12) 1-1,1-2,1-3
90	Ca++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
91	Ca++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
92	Ca++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
93	Ca++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
94	Ca++	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
95	Ca++	HPO4=	0.00000	0.00000	0.00000	0.00000	(1.4,12) 2-2
96	Ca++	PO4=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
97	Mg++	Cl-	0.35235	1.68150	0.00000	0.00519	(2.0,12) 1-1,1-2,1-3
98	Mg++	SO4=	0.22100	3.34300	-37.23000	0.02500	(1.4,12) 2-2
99	Mg++	HSO4-	0.47460	1.72900	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
100	Mg++	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
101	Mg++	HCO3-	0.32900	0.60720	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
102	Mg++	CO3=	0.00000	0.00000	0.00000	0.00000	(1.4,12) 2-2
103	Mg++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
104	Mg++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
105	Mg++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
106	Mg++	Br-	*0.00000*	*0.00000*	*0.00000*	*0.00000*	(2.0,12) 1-1,1-2,1-3
107	Mg++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
108	Mg++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
109	Mg++	ClO4-	0.49610	2.00800	0.00000	0.00958	(2.0,12) 1-1,1-2,1-3
110	Mg++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
111	Mg++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
112	Mg++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
113	Mg++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
114	Mg++	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
115	Mg++	HPO4=	0.00000	0.00000	0.00000	0.00000	(1.4,12) 2-2
116	Mg++	PO4=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
117	MgOH+	Cl-	-0.10000	1.65800	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
118	MgOH+	SO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
119	MgOH+	HSO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
120	MgOH+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
121	MgOH+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
122	MgOH+	CO3=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
123	MgOH+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
124	MgOH+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
125	MgOH+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
126	MgOH+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
127	MgOH+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
128	MgOH+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
129	MgOH+	ClO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
130	MgOH+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
131	MgOH+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
132	MgOH+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
133	MgOH+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
134	MgOH+	*H2PO4-*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	(2.0,12) 1-1,1-2,1-3
135	MgOH+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
136	MgOH+	PO4=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
137	H+	Cl-	0.17750	0.29450	0.00000	0.00080	(2.0,12) 1-1,1-2,1-3
138	H+	SO4=	0.02980	0.00000	0.00000	0.04380	(2.0,12) 1-1,1-2,1-3
139	H+	HSO4-	0.20650	0.55560	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
140	H+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
141	H+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
142	H+	CO3=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
143	H+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
144	H+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
145	H+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
146	H+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
147	H+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
148	H+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
149	H+	ClO4-	0.17470	0.29310	0.00000	0.00819	(2.0,12) 1-1,1-2,1-3
150	H+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
151	H+	*NpO2CO3-*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	(2.0,12) 1-1,1-2,1-3
152	H+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
153	H+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
154	H+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
155	H+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
156	H+	PO4=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
157	MgB(OH)4+	Cl-	0.16000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
158	MgB(OH)4+	SO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
159	MgB(OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
160	MgB(OH)4+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
161	MgB(OH)4+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
162	MgB(OH)4+	CO3=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
163	MgB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
164	MgB(OH)4+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
165	MgB(OH)4+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
166	MgB(OH)4+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
167	MgB(OH)4+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
168	MgB(OH)4+	*Am(CO3)3=-*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	(2.0,12) 1-1,1-2,1-3
169	MgB(OH)4+	ClO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
170	MgB(OH)4+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
171	MgB(OH)4+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
172	MgB(OH)4+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

173	MgB(OH)4+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
174	MgB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
175	MgB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
176	MgB(OH)4+	PO4=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
177	CaB(OH)4+	Cl-	0.12000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
178	CaB(OH)4+	SO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
179	CaB(OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
180	CaB(OH)4+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
181	CaB(OH)4+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
182	CaB(OH)4+	CO3=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
183	CaB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
184	CaB(OH)4+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
185	CaB(OH)4+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
186	CaB(OH)4+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
187	CaB(OH)4+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
188	CaB(OH)4+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
189	CaB(OH)4+	ClO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
190	CaB(OH)4+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
191	CaB(OH)4+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
192	CaB(OH)4+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
193	CaB(OH)4+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
194	CaB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
195	CaB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
196	CaB(OH)4+	PO4=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
197	Am+++	Cl-	0.61170	5.40300	0.00000	-0.02840	(2.0,12)	1-1,1-2,1-3
198	Am+++	SO4=	3.03980	0.00000	-2500.00000	0.00000	(1.4,50)	2-(n>2)
199	Am+++	HSO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
200	Am+++	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
201	Am+++	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
202	Am+++	CO3=	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
203	Am+++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
204	Am+++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
205	Am+++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
206	Am+++	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
207	Am+++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
208	Am+++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
209	Am+++	ClO4-	0.80000	5.35000	0.00000	-0.00480	(2.0,12)	1-1,1-2,1-3
210	Am+++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
211	Am+++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
212	Am+++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
213	Am+++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
214	Am+++	H2PO4-	0.00000	0.00000	-92.90000	0.00000	(2.0,12)	1-1,1-2,1-3
215	Am+++	HPO4=	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
216	Am+++	PO4=-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
217	AmCO3+	Cl-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
218	AmCO3+	SO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
219	AmCO3+	HSO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
220	AmCO3+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
221	AmCO3+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
222	AmCO3+	CO3=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
223	AmCO3+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
224	AmCO3+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
225	AmCO3+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
226	AmCO3+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
227	AmCO3+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
228	AmCO3+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
229	AmCO3+	ClO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
230	AmCO3+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
231	AmCO3+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
232	AmCO3+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
233	AmCO3+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
234	AmCO3+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
235	AmCO3+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
236	AmCO3+	PO4=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
237	Th++++	Cl-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
238	Th++++	SO4=	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
239	Th++++	HSO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
240	Th++++	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
241	Th++++	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
242	Th++++	CO3=	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
243	Th++++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
244	Th++++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
245	Th++++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
246	Th++++	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
247	Th++++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
248	Th++++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
249	Th++++	ClO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
250	Th++++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
251	Th++++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
252	Th++++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
253	Th++++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
254	Th++++	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
255	Th++++	HPO4=	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
256	Th++++	PO4=-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
257	UO2++	Cl-	0.42740	1.64400	0.00000	-0.03686	(2.0,12)	1-1,1-2,1-3
258	UO2++	SO4=	0.32200	1.82700	0.00000	-0.01760	(1.4,12)	2-2
259	UO2++	HSO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
260	UO2++	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
261	UO2++	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
262	UO2++	CO3=	0.00000	0.00000	0.00000	0.00000	(1.4,12)	2-2

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

UO2++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
UO2++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
UO2++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
UO2++	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
UO2++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
UO2++	Am(CO3)3=-	0.00000	0.00000	*0.00000*	*0.00000*	(1.4,50)	2-(n>2)
UO2++	ClO4-	0.61130	2.14400	0.00000	0.02168	(2.0,12)	1-1,1-2,1-3
UO2++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
UO2++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
UO2++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
UO2++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
UO2++	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
UO2++	HPO4=	0.00000	0.00000	0.00000	0.00000	(1.4,12)	2-2
UO2++	PO4=-	0.00000	0.00000	0.00000	0.00000	(1.4,50)	2-(n>2)
NpO2+	Cl-	0.16900	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	SO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	*HSO4-*	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	CO3=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	*B4O5(OH)4=*	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	ClO4-	0.31200	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	NpO2CO3-	*0.00000*	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
NpO2+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
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)

	K+	Ca++	Mg++	MgOH+	H+	MgB(OH)4+	CaB(OH)4+	Am+++	AmCO3+	Th++++
Na+	-0.01200	0.07000	0.07000	0.00000	0.03600	0.00000	0.00000	0.00000	0.00000	0.00000
	UO2++	NpO2+								
Na+	0.00000	0.00000								

	Ca++	Mg++	MgOH+	H+	MgB(OH)4+	CaB(OH)4+	Am+++	AmCO3+	Th++++	UO2++
K+	0.03200	0.00000	0.00000	0.00500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	NpO2+									
K+	0.00000									

	Mg++	MgOH+	H+	MgB(OH)4+	CaB(OH)4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+
Ca++	0.00700	0.00000	0.09200	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

	MgOH+	H+	MgB(OH)4+	CaB(OH)4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+
Mg++	0.00000	0.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

	H+	MgB(OH)4+	CaB(OH)4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+
MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

	MgB(OH)4+	CaB(OH)4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+
H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

	CaB(OH)4+	Am+++	AmCO3+	Th++++	UO2++	NpO2+
MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

	Am+++	AmCO3+	Th++++	UO2++	NpO2+
CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000

	AmCO3+	Th++++	UO2++	NpO2+
Am+++	0.00000	0.00000	0.00000	0.00000

	Th++++	UO2++	NpO2+
AmCO3+	*0.00000*	0.00000	0.00000

	UO2++	NpO2+
Th++++	0.00000	0.00000

	NpO2+
UO2++	*0.00000*

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

	SO4=	HSO4-	OH-	HCO3-	CO3=	B(OH)4-	B3O3(OH)4-	B4O5(OH)4=	Br-	Am(CO3)2-
Cl-	*0.02000*	*-0.00600*	*-0.05000*	*0.03000*	*-0.02000*	-0.06500	0.12000	0.07400	0.00000	0.00000
	Am(CO3)3=-	ClO4-	NpO2(OH)2-	NpO2CO3-	NpO2(CO3)2	NpO2(CO3)3	H2PO4-	HPO4=	PO4=-	
Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10000	0.00000	0.00000	

	HSO4-	OH-	HCO3-	CO3=	B(OH)4-	B3O3(OH)4-	B4O5(OH)4=	Br-	Am(CO3)2-	Am(CO3)3=-
SO4=	0.00000	-0.01300	0.01000	0.02000	-0.01200	0.10000	0.12000	0.00000	0.00000	0.00000
	ClO4-	NpO2(OH)2-	NpO2CO3-	NpO2(CO3)2	NpO2(CO3)3	H2PO4-	HPO4=	PO4=-		
SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

```
                  OH-         HCO3-       CO3=        B(OH)4-     B3O3(OH)4-  B4O5(OH)4=  Br-         Am(CO3)2-   Am(CO3)3=-  ClO4-
HSO4-             0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
                  NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
HSO4-             0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000

                  HCO3-       CO3=        B(OH)4-     B3O3(OH)4-  B4O5(OH)4=  Br-         Am(CO3)2-   Am(CO3)3=-  ClO4-       NpO2(OH)2-
OH-               0.00000     0.10000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
                  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
OH-               0.00000     0.00000     0.00000     0.00000     0.00000     0.00000

                  CO3=        B(OH)4-     B3O3(OH)4-  B4O5(OH)4=  Br-         Am(CO3)2-   Am(CO3)3=-  ClO4-       NpO2(OH)2-  NpO2CO3-
HCO3-            -0.04000     0.00000    -0.10000    -0.08700     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
                  NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
HCO3-             0.00000     0.00000     0.00000     0.00000     0.00000

                  B(OH)4-     B3O3(OH)4-  B4O5(OH)4=  Br-         Am(CO3)2-   Am(CO3)3=-  ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2
CO3=              0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
                  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
CO3=              0.00000     0.00000     0.00000     0.00000

                  B3O3(OH)4-  B4O5(OH)4=  Br-         Am(CO3)2-   Am(CO3)3=-  ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3
B(OH)4-           0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
                  H2PO4-      HPO4=       PO4=-
B(OH)4-           0.00000     0.00000     0.00000

                  B4O5(OH)4=  Br-         Am(CO3)2-   Am(CO3)3=-  ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-
B3O3(OH)4-        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
                  HPO4=       PO4=-
B3O3(OH)4-        0.00000     0.00000

                  Br-         Am(CO3)2-   Am(CO3)3=-  ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=
B4O5(OH)4=        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
                  PO4=-
B4O5(OH)4=        0.00000

                  Am(CO3)2-   Am(CO3)3=-  ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
Br-               0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000

                  Am(CO3)3=-  ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
Am(CO3)2-         0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000

                  ClO4-       NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
Am(CO3)3=-        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000

                  NpO2(OH)2-  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
ClO4-             0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000

                  NpO2CO3-    NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
NpO2(OH)2-        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000

                  NpO2(CO3)2  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
NpO2CO3-          0.00000     0.00000     0.00000     0.00000     0.00000

                  NpO2(CO3)3  H2PO4-      HPO4=       PO4=-
NpO2(CO3)2=-      0.00000     0.00000     0.00000     0.00000

                  H2PO4-      HPO4=       PO4=-
NpO2(CO3)3=--     0.00000     0.00000     0.00000

                  HPO4=       PO4=-
H2PO4-            0.00000     0.00000

                  PO4=-
HPO4=             0.00000

Cation-Cation-Anion Ternary Interactions:  psi(,,,)

                                Cl-         SO4=        HSO4-       OH-         HCO3-       CO3=        B(OH)4-     B3O3(OH)4   B4O5(OH)4   Br-
Na+               K+           -0.00180    -0.01000     0.00000     0.00000    -0.00300     0.00300     0.00000     0.00000     0.00000     0.00000
Na+               Ca++         -0.00700    -0.05500     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               Mg++         -0.01200    -0.01500     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               MgOH+         0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               H+           -0.00400     0.00000    -0.01290     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               MgB(OH)4+     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               CaB(OH)4+     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               Am+++         0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               AmCO3+        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               Th++++        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               UO2++         0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Na+               NpO2+         0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                Ca++         -0.02500     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                Mg++         -0.02200    -0.04800     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                MgOH+         0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                H+           -0.01100     0.19700    -0.02650     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                MgB(OH)4+     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                CaB(OH)4+     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                Am+++         0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                AmCO3+        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
K+                Th++++        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
```

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

443	K+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
444	K+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
445	Ca++	Mg++	-0.01200	0.02400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
446	Ca++	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
447	Ca++	H+	-0.01500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
448	Ca++	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
449	Ca++	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
450	Ca++	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
451	Ca++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
452	Ca++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
453	Ca++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
454	Ca++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
455	Mg++	MgOH+	0.02800	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
456	Mg++	H+	-0.01100	0.00000	-0.01780	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
457	Mg++	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
458	Mg++	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
459	Mg++	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
460	Mg++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
461	Mg++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
462	Mg++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
463	Mg++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
464	MgOH+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
465	MgOH+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
466	MgOH+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
467	MgOH+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
468	MgOH+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
469	MgOH+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
470	MgOH+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
471	MgOH+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
472	H+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
473	H+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
474	H+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
475	H+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
476	H+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
477	H+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
478	H+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
479	MgB(OH)4+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
480	MgB(OH)4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
481	MgB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
482	MgB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
483	MgB(OH)4+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
484	MgB(OH)4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
485	CaB(OH)4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
486	CaB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
487	CaB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
488	CaB(OH)4+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
489	CaB(OH)4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
490	Am+++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
491	Am+++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
492	Am+++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
493	Am+++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
494	AmCO3+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
495	AmCO3+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
496	AmCO3+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
497	Th++++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
498	Th++++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
499	UO2++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
500												
501			Am(CO3)2-	Am(CO3)3=	ClO4-	NpO2(OH)2	NpO2CO3-	NpO2(CO3)	NpO2(CO3)	H2PO4-	HPO4=	PO4=-
502	Na+	K+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
503	Na+	Ca++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
504	Na+	Mg++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
505	Na+	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
506	Na+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
507	Na+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
508	Na+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
509	Na+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
510	Na+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
511	Na+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
512	Na+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
513	Na+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
514	K+	Ca++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
515	K+	Mg++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
516	K+	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
517	K+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
518	K+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
519	K+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
520	K+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
521	K+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
522	K+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
523	K+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
524	K+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
525	Ca++	Mg++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
526	Ca++	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
527	Ca++	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
528	Ca++	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
529	Ca++	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
530	Ca++	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
531	Ca++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
532	Ca++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

533	Ca++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
534	Ca++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
535	Mg++	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
536	Mg++	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
537	Mg++	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
538	Mg++	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
539	Mg++	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
540	Mg++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
541	Mg++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
542	Mg++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
543	Mg++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
544	MgOH+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
545	MgOH+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
546	MgOH+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
547	MgOH+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
548	MgOH+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
549	MgOH+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
550	MgOH+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
551	MgOH+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
552	H+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
553	H+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
554	H+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
555	H+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
556	H+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
557	H+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
558	H+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
559	MgB(OH)4+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
560	MgB(OH)4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
561	MgB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
562	MgB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
563	MgB(OH)4+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
564	MgB(OH)4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
565	CaB(OH)4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
566	CaB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
567	CaB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
568	CaB(OH)4+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
569	CaB(OH)4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
570	Am+++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
571	Am+++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
572	Am+++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
573	Am+++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
574	AmCO3+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
575	AmCO3+	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
576	AmCO3+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
577	Th++++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
578	Th++++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
579	UO2++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

580

581 Anion-Anion-Cation Ternary Interactions: psi(,,)

582

			Na+	K+	Ca++	Mg++	MgOH+	H+	MgB(OH)4+	CaB(OH)4+	Am+++	AmCO3+
583	Cl-	SO4=	0.00140	0.00000	-0.01800	-0.00400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
584	Cl-	HSO4-	-0.00600	0.00000	0.00000	0.00000	0.00000	0.01300	0.00000	0.00000	0.00000	0.00000
585	Cl-	OH-	-0.00600	-0.00600	-0.02500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
586	Cl-	HCO3-	-0.01500	0.00000	0.00000	-0.09600	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
587	Cl-	CO3=	0.00850	0.00400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
588	Cl-	B(OH)4-	-0.00730	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
589	Cl-	B3O3(OH)4-	-0.02400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
590	Cl-	B4O5(OH)4=	0.02600	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
591	Cl-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
592	Cl-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
593	Cl-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
594	Cl-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
595	Cl-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
596	Cl-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
597	Cl-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
598	Cl-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
599	Cl-	H2PO4-	0.00000	-0.01000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
600	Cl-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
601	Cl-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
602	SO4=	HSO4-	-0.00940	-0.06770	0.00000	-0.04250	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
603	SO4=	OH-	-0.00900	-0.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
604	SO4=	HCO3-	-0.00500	0.00000	0.00000	-0.16100	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
605	SO4=	CO3=	-0.00500	-0.00900	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
606	SO4=	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
607	SO4=	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
608	SO4=	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
609	SO4=	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
610	SO4=	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
611	SO4=	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
612	SO4=	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
613	SO4=	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
614	SO4=	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
615	SO4=	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
616	SO4=	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
617	SO4=	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
618	SO4=	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
619	SO4=	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
620	HSO4-	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
621	HSO4-	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

623	HSO4-	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
624	HSO4-	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
625	HSO4-	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
626	HSO4-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
627	HSO4-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
628	HSO4-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
629	HSO4-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
630	HSO4-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
631	HSO4-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
632	HSO4-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
633	HSO4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
634	HSO4-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
635	HSO4-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
636	HSO4-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
637	HSO4-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
638	OH-	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
639	OH-	CO3=	-0.01700	-0.01000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
640	OH-	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
641	OH-	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
642	OH-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
643	OH-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
644	OH-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
645	OH-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
646	OH-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
647	OH-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
648	OH-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
649	OH-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
650	OH-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
651	OH-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
652	OH-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
653	OH-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
654	HCO3-	CO3=	0.00200	0.01200	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
655	HCO3-	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
656	HCO3-	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
657	HCO3-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
658	HCO3-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
659	HCO3-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
660	HCO3-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
661	HCO3-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
662	HCO3-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
663	HCO3-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
664	HCO3-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
665	HCO3-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
666	HCO3-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
667	HCO3-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
668	HCO3-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
669	CO3=	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
670	CO3=	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
671	CO3=	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
672	CO3=	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
673	CO3=	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
674	CO3=	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
675	CO3=	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
676	CO3=	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
677	CO3=	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
678	CO3=	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
679	CO3=	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
680	CO3=	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
681	CO3=	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
682	CO3=	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
683	B(OH)4-	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
684	B(OH)4-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
685	B(OH)4-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
686	B(OH)4-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
687	B(OH)4-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
688	B(OH)4-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
689	B(OH)4-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
690	B(OH)4-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
691	B(OH)4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
692	B(OH)4-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
693	B(OH)4-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
694	B(OH)4-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
695	B(OH)4-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
696	B3O3(OH)4-	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
697	B3O3(OH)4-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
698	B3O3(OH)4-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
699	B3O3(OH)4-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
700	B3O3(OH)4-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
701	B3O3(OH)4-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
702	B3O3(OH)4-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
703	B3O3(OH)4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
704	B3O3(OH)4-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
705	B3O3(OH)4-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
706	B3O3(OH)4-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
707	B3O3(OH)4-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
708	B4O5(OH)4=	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
709	B4O5(OH)4=	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
710	B4O5(OH)4=	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
711	B4O5(OH)4=	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
712	B4O5(OH)4=	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

713	B4O5(OH)4=	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
714	B4O5(OH)4=	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
715	B4O5(OH)4=	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
716	B4O5(OH)4=	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
717	B4O5(OH)4=	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
718	B4O5(OH)4=	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
719	Br-	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
720	Br-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
721	Br-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
722	Br-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
723	Br-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
724	Br-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
725	Br-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
726	Br-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
727	Br-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
728	Br-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
729	Am(CO3)2-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
730	Am(CO3)2-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
731	Am(CO3)2-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
732	Am(CO3)2-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
733	Am(CO3)2-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
734	Am(CO3)2-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
735	Am(CO3)2-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
736	Am(CO3)2-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
737	Am(CO3)2-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
738	Am(CO3)3=-	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
739	Am(CO3)3=-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
740	Am(CO3)3=-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
741	Am(CO3)3=-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
742	Am(CO3)3=-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
743	Am(CO3)3=-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
744	Am(CO3)3=-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
745	Am(CO3)3=-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
746	ClO4-	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
747	ClO4-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
748	ClO4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
749	ClO4-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
750	ClO4-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
751	ClO4-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
752	ClO4-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
753	NpO2(OH)2-	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
754	NpO2(OH)2-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
755	NpO2(OH)2-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
756	NpO2(OH)2-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
757	NpO2(OH)2-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
758	NpO2(OH)2-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
759	NpO2CO3-	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
760	NpO2CO3-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
761	NpO2CO3-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
762	NpO2CO3-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
763	NpO2CO3-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
764	NpO2(CO3)2=-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
765	NpO2(CO3)2=-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
766	NpO2(CO3)2=-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
767	NpO2(CO3)2=-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
768	NpO2(CO3)3==-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
769	NpO2(CO3)3==-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
770	NpO2(CO3)3==-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
771	H2PO4-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
772	H2PO4-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
773	HPO4=	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
774												
775			Th++++	UO2++	NpO2+							
776	Cl-	SO4=	0.00000	0.00000	0.00000							
777	Cl-	HSO4-	0.00000	0.00000	0.00000							
778	Cl-	OH-	0.00000	0.00000	0.00000							
779	Cl-	HCO3-	0.00000	0.00000	0.00000							
780	Cl-	CO3=	0.00000	0.00000	0.00000							
781	Cl-	B(OH)4-	0.00000	0.00000	0.00000							
782	Cl-	B3O3(OH)4-	0.00000	0.00000	0.00000							
783	Cl-	B4O5(OH)4=	0.00000	0.00000	0.00000							
784	Cl-	Br-	0.00000	0.00000	0.00000							
785	Cl-	Am(CO3)2-	0.00000	0.00000	0.00000							
786	Cl-	Am(CO3)3=-	0.00000	0.00000	0.00000							
787	Cl-	ClO4-	0.00000	0.00000	0.00000							
788	Cl-	NpO2(OH)2-	0.00000	0.00000	0.00000							
789	Cl-	NpO2CO3-	0.00000	0.00000	0.00000							
790	Cl-	NpO2(CO3)2=-	0.00000	0.00000	0.00000							
791	Cl-	NpO2(CO3)3==-	0.00000	0.00000	0.00000							
792	Cl-	H2PO4-	0.00000	0.00000	0.00000							
793	Cl-	HPO4=	0.00000	0.00000	0.00000							
794	Cl-	PO4=-	0.00000	0.00000	0.00000							
795	SO4=	HSO4-	0.00000	0.00000	0.00000							
796	SO4=	OH-	0.00000	0.00000	0.00000							
797	SO4=	HCO3-	0.00000	0.00000	0.00000							
798	SO4=	CO3=	0.00000	0.00000	0.00000							
799	SO4=	B(OH)4-	0.00000	0.00000	0.00000							
800	SO4=	B3O3(OH)4-	0.00000	0.00000	0.00000							
801	SO4=	B4O5(OH)4=	0.00000	0.00000	0.00000							
802	SO4=	Br-	0.00000	0.00000	0.00000							

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

803	SO4=	Am(CO3)2-	0.00000	0.00000	0.00000
804	SO4=	Am(CO3)3=-	0.00000	0.00000	0.00000
805	SO4=	ClO4-	0.00000	0.00000	0.00000
806	SO4=	NpO2(OH)2-	0.00000	0.00000	0.00000
807	SO4=	NpO2CO3-	0.00000	0.00000	0.00000
808	SO4=	NpO2(CO3)2=-	0.00000	0.00000	0.00000
809	SO4=	NpO2(CO3)3==-	0.00000	0.00000	0.00000
810	SO4=	H2PO4-	0.00000	0.00000	0.00000
811	SO4=	HPO4=	0.00000	0.00000	0.00000
812	SO4=	PO4=-	0.00000	0.00000	0.00000
813	HSO4-	OH-	0.00000	0.00000	0.00000
814	HSO4-	HCO3-	0.00000	0.00000	0.00000
815	HSO4-	CO3=	0.00000	0.00000	0.00000
816	HSO4-	B(OH)4-	0.00000	0.00000	0.00000
817	HSO4-	B3O3(OH)4-	0.00000	0.00000	0.00000
818	HSO4-	B4O5(OH)4=	0.00000	0.00000	0.00000
819	HSO4-	Br-	0.00000	0.00000	0.00000
820	HSO4-	Am(CO3)2-	0.00000	0.00000	0.00000
821	HSO4-	Am(CO3)3=-	0.00000	0.00000	0.00000
822	HSO4-	ClO4-	0.00000	0.00000	0.00000
823	HSO4-	NpO2(OH)2-	0.00000	0.00000	0.00000
824	HSO4-	NpO2CO3-	0.00000	0.00000	0.00000
825	HSO4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
826	HSO4-	NpO2(CO3)3==-	0.00000	0.00000	0.00000
827	HSO4-	H2PO4-	0.00000	0.00000	0.00000
828	HSO4-	HPO4=	0.00000	0.00000	0.00000
829	HSO4-	PO4=-	0.00000	0.00000	0.00000
830	OH-	HCO3-	0.00000	0.00000	0.00000
831	OH-	CO3=	0.00000	0.00000	0.00000
832	OH-	B(OH)4-	0.00000	0.00000	0.00000
833	OH-	B3O3(OH)4-	0.00000	0.00000	0.00000
834	OH-	B4O5(OH)4=	0.00000	0.00000	0.00000
835	OH-	Br-	0.00000	0.00000	0.00000
836	OH-	Am(CO3)2-	0.00000	0.00000	0.00000
837	OH-	Am(CO3)3=-	0.00000	0.00000	0.00000
838	OH-	ClO4-	0.00000	0.00000	0.00000
839	OH-	NpO2(OH)2-	0.00000	0.00000	0.00000
840	OH-	NpO2CO3-	0.00000	0.00000	0.00000
841	OH-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
842	OH-	NpO2(CO3)3==-	0.00000	0.00000	0.00000
843	OH-	H2PO4-	0.00000	0.00000	0.00000
844	OH-	HPO4=	0.00000	0.00000	0.00000
845	OH-	PO4=-	0.00000	0.00000	0.00000
846	HCO3-	CO3=	0.00000	0.00000	0.00000
847	HCO3-	B(OH)4-	0.00000	0.00000	0.00000
848	HCO3-	B3O3(OH)4-	0.00000	0.00000	0.00000
849	HCO3-	B4O5(OH)4=	0.00000	0.00000	0.00000
850	HCO3-	Br-	0.00000	0.00000	0.00000
851	HCO3-	Am(CO3)2-	0.00000	0.00000	0.00000
852	HCO3-	Am(CO3)3=-	0.00000	0.00000	0.00000
853	HCO3-	ClO4-	0.00000	0.00000	0.00000
854	HCO3-	NpO2(OH)2-	0.00000	0.00000	0.00000
855	HCO3-	NpO2CO3-	0.00000	0.00000	0.00000
856	HCO3-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
857	HCO3-	NpO2(CO3)3==-	0.00000	0.00000	0.00000
858	HCO3-	H2PO4-	0.00000	0.00000	0.00000
859	HCO3-	HPO4=	0.00000	0.00000	0.00000
860	HCO3-	PO4=-	0.00000	0.00000	0.00000
861	CO3=	B(OH)4-	0.00000	0.00000	0.00000
862	CO3=	B3O3(OH)4-	0.00000	0.00000	0.00000
863	CO3=	B4O5(OH)4=	0.00000	0.00000	0.00000
864	CO3=	Br-	0.00000	0.00000	0.00000
865	CO3=	Am(CO3)2-	0.00000	0.00000	0.00000
866	CO3=	Am(CO3)3=-	0.00000	0.00000	0.00000
867	CO3=	ClO4-	0.00000	0.00000	0.00000
868	CO3=	NpO2(OH)2-	0.00000	0.00000	0.00000
869	CO3=	NpO2CO3-	0.00000	0.00000	0.00000
870	CO3=	NpO2(CO3)2=-	0.00000	0.00000	0.00000
871	CO3=	NpO2(CO3)3==-	0.00000	0.00000	0.00000
872	CO3=	H2PO4-	0.00000	0.00000	0.00000
873	CO3=	HPO4=	0.00000	0.00000	0.00000
874	CO3=	PO4=-	0.00000	0.00000	0.00000
875	B(OH)4-	B3O3(OH)4-	0.00000	0.00000	0.00000
876	B(OH)4-	B4O5(OH)4=	0.00000	0.00000	0.00000
877	B(OH)4-	Br-	0.00000	0.00000	0.00000
878	B(OH)4-	Am(CO3)2-	0.00000	0.00000	0.00000
879	B(OH)4-	Am(CO3)3=-	0.00000	0.00000	0.00000
880	B(OH)4-	ClO4-	0.00000	0.00000	0.00000
881	B(OH)4-	NpO2(OH)2-	0.00000	0.00000	0.00000
882	B(OH)4-	NpO2CO3-	0.00000	0.00000	0.00000
883	B(OH)4-	NpO2(CO3)2=-	0.00000	0.00000	0.00000
884	B(OH)4-	NpO2(CO3)3==-	0.00000	0.00000	0.00000
885	B(OH)4-	H2PO4-	0.00000	0.00000	0.00000
886	B(OH)4-	HPO4=	0.00000	0.00000	0.00000
887	B(OH)4-	PO4=-	0.00000	0.00000	0.00000
888	B3O3(OH)4-	B4O5(OH)4=	0.00000	0.00000	0.00000
889	B3O3(OH)4-	Br-	0.00000	0.00000	0.00000
890	B3O3(OH)4-	Am(CO3)2-	0.00000	0.00000	0.00000
891	B3O3(OH)4-	Am(CO3)3=-	0.00000	0.00000	0.00000
892	B3O3(OH)4-	ClO4-	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

```
B3O3(OH)4-      NpO2(OH)2-      0.00000   0.00000   0.00000
B3O3(OH)4-      NpO2CO3-        0.00000   0.00000   0.00000
B3O3(OH)4-      NpO2(CO3)2=-    0.00000   0.00000   0.00000
B3O3(OH)4-      NpO2(CO3)3=3-   0.00000   0.00000   0.00000
B3O3(OH)4-      H2PO4-          0.00000   0.00000   0.00000
B3O3(OH)4-      HPO4=           0.00000   0.00000   0.00000
B3O3(OH)4-      PO4=-           0.00000   0.00000   0.00000
B4O5(OH)4=      Br-             0.00000   0.00000   0.00000
B4O5(OH)4=      Am(CO3)2-       0.00000   0.00000   0.00000
B4O5(OH)4=      Am(CO3)3=-      0.00000   0.00000   0.00000
B4O5(OH)4=      ClO4-           0.00000   0.00000   0.00000
B4O5(OH)4=      NpO2(OH)2-      0.00000   0.00000   0.00000
B4O5(OH)4=      NpO2CO3-        0.00000   0.00000   0.00000
B4O5(OH)4=      NpO2(CO3)2=-    0.00000   0.00000   0.00000
B4O5(OH)4=      NpO2(CO3)3=3-   0.00000   0.00000   0.00000
B4O5(OH)4=      H2PO4-          0.00000   0.00000   0.00000
B4O5(OH)4=      HPO4=           0.00000   0.00000   0.00000
B4O5(OH)4=      PO4=-           0.00000   0.00000   0.00000
Br-             Am(CO3)2-       0.00000   0.00000   0.00000
Br-             Am(CO3)3=-      0.00000   0.00000   0.00000
Br-             ClO4-           0.00000   0.00000   0.00000
Br-             NpO2(OH)2-      0.00000   0.00000   0.00000
Br-             NpO2CO3-        0.00000   0.00000   0.00000
Br-             NpO2(CO3)2=-    0.00000   0.00000   0.00000
Br-             NpO2(CO3)3=3-   0.00000   0.00000   0.00000
Br-             H2PO4-          0.00000   0.00000   0.00000
Br-             HPO4=           0.00000   0.00000   0.00000
Br-             PO4=-           0.00000   0.00000   0.00000
Am(CO3)2-       Am(CO3)3=-      0.00000   0.00000   0.00000
Am(CO3)2-       ClO4-           0.00000   0.00000   0.00000
Am(CO3)2-       NpO2(OH)2-      0.00000   0.00000   0.00000
Am(CO3)2-       NpO2CO3-        0.00000   0.00000   0.00000
Am(CO3)2-       NpO2(CO3)2=-    0.00000   0.00000   0.00000
Am(CO3)2-       NpO2(CO3)3=3-   0.00000   0.00000   0.00000
Am(CO3)2-       H2PO4-          0.00000   0.00000   0.00000
Am(CO3)2-       HPO4=           0.00000   0.00000   0.00000
Am(CO3)2-       PO4=-           0.00000   0.00000   0.00000
Am(CO3)3=-      ClO4-           0.00000   0.00000   0.00000
Am(CO3)3=-      NpO2(OH)2-      0.00000   0.00000   0.00000
Am(CO3)3=-      NpO2CO3-        0.00000   0.00000   0.00000
Am(CO3)3=-      NpO2(CO3)2=-    0.00000   0.00000   0.00000
Am(CO3)3=-      NpO2(CO3)3=3-   0.00000   0.00000   0.00000
Am(CO3)3=-      H2PO4-          0.00000   0.00000   0.00000
Am(CO3)3=-      HPO4=           0.00000   0.00000   0.00000
Am(CO3)3=-      PO4=-           0.00000   0.00000   0.00000
ClO4-           NpO2(OH)2-      0.00000   0.00000   0.00000
ClO4-           NpO2CO3-        0.00000   0.00000   0.00000
ClO4-           NpO2(CO3)2=-    0.00000   0.00000   0.00000
ClO4-           NpO2(CO3)3=3-   0.00000   0.00000   0.00000
ClO4-           H2PO4-          0.00000   0.00000   0.00000
ClO4-           HPO4=           0.00000   0.00000   0.00000
ClO4-           PO4=-           0.00000   0.00000   0.00000
NpO2(OH)2-      NpO2CO3-        0.00000   0.00000   0.00000
NpO2(OH)2-      NpO2(CO3)2=-    0.00000   0.00000   0.00000
NpO2(OH)2-      NpO2(CO3)3=3-   0.00000   0.00000   0.00000
NpO2(OH)2-      H2PO4-          0.00000   0.00000   0.00000
NpO2(OH)2-      HPO4=           0.00000   0.00000   0.00000
NpO2(OH)2-      PO4=-           0.00000   0.00000   0.00000
NpO2CO3-        NpO2(CO3)2=-    0.00000   0.00000   0.00000
NpO2CO3-        NpO2(CO3)3=3-   0.00000   0.00000   0.00000
NpO2CO3-        H2PO4-          0.00000   0.00000   0.00000
NpO2CO3-        HPO4=           0.00000   0.00000   0.00000
NpO2CO3-        PO4=-           0.00000   0.00000   0.00000
NpO2(CO3)2=-    NpO2(CO3)3=3-   0.00000   0.00000   0.00000
NpO2(CO3)2=-    H2PO4-          0.00000   0.00000   0.00000
NpO2(CO3)2=-    HPO4=           0.00000   0.00000   0.00000
NpO2(CO3)2=-    PO4=-           0.00000   0.00000   0.00000
NpO2(CO3)3=3-   H2PO4-          0.00000   0.00000   0.00000
NpO2(CO3)3=3-   HPO4=           0.00000   0.00000   0.00000
NpO2(CO3)3=3-   PO4=-           0.00000   0.00000   0.00000
H2PO4-          HPO4=           0.00000   0.00000   0.00000
H2PO4-          PO4=-           0.00000   0.00000   0.00000
HPO4=           PO4=-           0.00000   0.00000   0.00000

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

                CO2(aq)    CaCO3(aq)  MgCO3(aq)  B(OH)3(aq) NpO2OH(aq) H3PO4(aq)
Na+             0.10000    0.00000    0.00000    -0.09700   0.00000    0.00000
K+              0.05100    0.00000    0.00000    -0.14000   0.00000   -0.07000
Ca++            0.18300    0.00000    0.00000     0.00000   0.00000    0.00000
Mg++            0.18300    0.00000    0.00000     0.00000   0.00000    0.00000
MgOH+           0.00000    0.00000    0.00000     0.00000   0.00000    0.00000
H+              0.00000    0.00000    0.00000     0.00000   0.00000    0.29000
MgB(OH)4+       0.00000    0.00000    0.00000     0.00000   0.00000    0.00000
CaB(OH)4+       0.00000    0.00000    0.00000     0.00000   0.00000    0.00000
Am+++           0.00000    0.00000    0.00000     0.00000   0.00000    0.00000
AmCO3+          0.00000    0.00000    0.00000     0.00000   0.00000    0.00000
Th++++          0.00000    0.00000    0.00000     0.00000   0.00000    0.00000
UO2++           0.00000    0.00000    0.00000     0.00000   0.00000    0.00000
NpO2+           0.00000    0.00000    0.00000     0.00000   0.00000    0.00000
```

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

Neutral- Anion Binary Interactions: lambda(n,a)

	CO2(aq)	CaCO3(aq)	MgCO3(aq)	B(OH)3(aq)	NpO2OH(aq)	H3PO4(aq)
Cl-	-0.00500	0.00000	0.00000	0.09100	0.00000	0.00000
SO4=	0.09700	0.00000	0.00000	0.01800	0.00000	0.00000
HSO4-	-0.00300	0.00000	0.00000	0.00000	0.00000	0.00000
OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
B3O3(OH)4-	0.00000	0.00000	0.00000	-0.20000	0.00000	0.00000
B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	-0.40000
HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Neutral-Cation-Anion Ternary Interactions: zeta(n,c,a)

		CO2(aq)	CaCO3(aq)	MgCO3(aq)	B(OH)3(aq	NpO2OH(aq	H3PO4(aq)
Na+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	SO4=	0.00000	0.00000	0.00000	0.04600	0.00000	0.00000
Na+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Na+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
K+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ca++	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

1073	Mg++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1074	Mg++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1075	Mg++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1076	Mg++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1077	Mg++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1078	Mg++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1079	Mg++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1080	Mg++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1081	Mg++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1082	Mg++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1083	Mg++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1084	Mg++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1085	Mg++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1086	Mg++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1087	Mg++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1088	Mg++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1089	Mg++	*NpO2(CO3)3==-*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	*0.00000*
1090	Mg++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1091	Mg++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1092	Mg++	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1093	MgOH+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1094	MgOH+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1095	MgOH+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1096	MgOH+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1097	MgOH+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1098	MgOH+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1099	MgOH+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1100	MgOH+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1101	MgOH+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1102	MgOH+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1103	MgOH+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1104	MgOH+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1105	MgOH+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1106	MgOH+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1107	MgOH+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1108	MgOH+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1109	MgOH+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1110	MgOH+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1111	MgOH+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1112	MgOH+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1113	H+	Cl-	0.00000	0.00000	0.00000	-0.01020	0.00000	0.00000
1114	H+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1115	H+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1116	H+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1117	H+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1118	H+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1119	H+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1120	H+	*B3O3(OH)4-*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	*0.00000*
1121	H+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1122	H+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1123	H+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1124	H+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1125	H+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1126	H+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1127	H+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1128	H+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1129	H+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1130	H+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1131	H+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1132	H+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1133	MgB(OH)4+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1134	MgB(OH)4+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1135	MgB(OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1136	MgB(OH)4+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1137	MgB(OH)4+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1138	MgB(OH)4+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1139	MgB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1140	MgB(OH)4+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1141	MgB(OH)4+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1142	MgB(OH)4+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1143	MgB(OH)4+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1144	MgB(OH)4+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1145	MgB(OH)4+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1146	MgB(OH)4+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1147	MgB(OH)4+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1148	MgB(OH)4+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1149	MgB(OH)4+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1150	MgB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1151	*MgB(OH)4+*	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1152	MgB(OH)4+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1153	CaB(OH)4+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1154	CaB(OH)4+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1155	CaB(OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1156	CaB(OH)4+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1157	CaB(OH)4+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1158	CaB(OH)4+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1159	CaB(OH)4+	*B(OH)4-*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	*0.00000*	*0.00000*
1160	CaB(OH)4+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1161	CaB(OH)4+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1162	CaB(OH)4+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

1153	CaB(OH)4+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1154	CaB(OH)4+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1155	CaB(OH)4+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1156	CaB(OH)4+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1157	CaB(OH)4+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1158	CaB(OH)4+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1159	CaB(OH)4+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1160	CaB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1161	CaB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1162	CaB(OH)4+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1163	Am+++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1164	Am+++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1165	Am+++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1166	Am+++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1167	Am+++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1168	Am+++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1169	Am+++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1170	Am+++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1171	Am+++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1172	Am+++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1173	Am+++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1174	Am+++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1175	Am+++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1176	Am+++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1177	Am+++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1178	Am+++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1179	Am+++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1180	Am+++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1181	Am+++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1182	Am+++	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1183	AmCO3+	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1184	AmCO3+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1185	AmCO3+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1186	AmCO3+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1187	AmCO3+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1188	AmCO3+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1189	AmCO3+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1200	AmCO3+	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1201	AmCO3+	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1202	AmCO3+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1203	AmCO3+	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1204	AmCO3+	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1205	AmCO3+	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1206	AmCO3+	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1207	AmCO3+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1208	AmCO3+	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1209	AmCO3+	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1210	AmCO3+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1211	AmCO3+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1212	AmCO3+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1213	Th++++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1214	Th++++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1215	Th++++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1216	Th++++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1217	Th++++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1218	Th++++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1219	Th++++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1220	Th++++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1221	Th++++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1222	Th++++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1223	Th++++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1224	Th++++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1225	Th++++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1226	Th++++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1227	Th++++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1228	Th++++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1229	Th++++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1230	Th++++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1231	Th++++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1232	Th++++	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1233	UO2++	Cl-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1234	UO2++	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1235	UO2++	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1236	UO2++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1237	UO2++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1238	UO2++	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1239	UO2++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1240	UO2++	B3O3(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1241	UO2++	B4O5(OH)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1242	UO2++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1243	UO2++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1244	UO2++	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1245	UO2++	ClO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1246	UO2++	NpO2(OH)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1247	UO2++	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1248	UO2++	NpO2(CO3)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1249	UO2++	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1250	UO2++	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1251	UO2++	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1252	UO2++	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

```
NpO2+           Cl-             0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           SO4=            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           HSO4-           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           OH-             0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           HCO3-           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           CO3=            0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           B(OH)4-         0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           B3O3(OH)4-      0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           B4O5(OH)4=      0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           Br-             0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           Am(CO3)2-       0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           Am(CO3)3=-      0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           ClO4-           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           NpO2(OH)2-      0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           NpO2CO3-        0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           NpO2(CO3)2=-    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           NpO2(CO3)3=3-   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           H2PO4-          0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
NpO2+           HPO4=           0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
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


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


 115 Species                      23 Elements

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


    Species Name                          Phase          Mol.Wt.     Std Chemical Potential, u/RT
  1 H2O                          WATER    aqueous         18.015       -95.663
  2 Na+                            Na+    aqueous         22.990      -105.651
  3 K+                              K+    aqueous         39.098      -113.957
  4 Ca++                           Ca++    aqueous         40.080      -223.300
  5 Mg++                           Mg++    aqueous         24.305      -183.468
  6 MgOH+                         MgOH+    aqueous         41.312      -251.940
  7 H+                              H+    aqueous          1.008         0.000
  8 Cl-                             Cl-   aqueous         35.453       -52.955
  9 SO4=                           SO4=    aqueous         96.058      -300.386
 10 HSO4-                         HSO4-    aqueous         97.066      -304.942
 11 OH-                           OH-      aqueous         17.007       -63.435
 12 HCO3-                         HCO3-    aqueous         61.017      -236.751
 13 CO3=                          CO3=     aqueous         60.009      -212.944
 14 CO2(aq)                     CO2(aq)    aqueous         44.010      -155.680
 15 CaCO3(aq)                 CaCO3(aq)    aqueous        100.089      -443.500
 16 MgCO3(aq)                 MgCO3(aq)    aqueous         84.314      -403.155
 17 B(OH)3(aq)                B(OH)3(aq)   aqueous         61.832      -390.810
 18 B(OH)4-                     B(OH)4-    aqueous         78.839      -465.200
 19 B3O3(OH)4-                B3O3(OH)4-   aqueous        148.457      -963.770
 20 B4O5(OH)4=                B4O5(OH)4=   aqueous        191.266     -1239.100
 21 CaB(OH)4+                   CaB(OH)4+  aqueous        118.919      -692.300
 22 MgB(OH)4+                   MgB(OH)4+  aqueous        103.144      -651.890
 23 Br-                           Br-      aqueous         79.904      -999.990
 24 ClO4-              perchlorate ClO4-   aqueous         99.451      -999.990
 25 NaOH(aq).....to.titrate.base.only       aqueous         39.997       500.000
 26 HCl(aq).....to.titrate.acid.only        aqueous         36.461       500.000
 27 HClO4(aq).....to.titrate.acid.only      aqueous        100.459       500.000
 28 PosIon.............POSITIVE.ION        aqueous          0.000         0.000
 29 NegIon.............NEGATIVE.ION        aqueous          0.000         0.000
 30 PosIon(OH)(aq).....to.titrate.base      aqueous         17.007       500.000
```

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

31	HNegIon(aq).....to.titrate.acid	aqueous	1.008	500.000
32	*Tracer(aq).....conservative.tracer*	aqueous	0.000	0.000
33	H3PO4(aq) H3PO4(aq)	aqueous	97.995	-460.900
34	H2PO4- H2PO4-	aqueous	96.987	-455.960
35	HPO4= HPO4=	aqueous	95.980	-439.367
36	PO4=- PO4=-	aqueous	94.972	-410.947
37	NpO2+ NpO2+	aqueous	269.047	-369.127
38	NpO2OH(aq) NpO2OH(aq)	aqueous	286.054	-438.518
39	NpO2(OH)2- NpO2(OH)2-	aqueous	303.062	-505.829
40	NpO2CO3- NpO2CO3-	aqueous	329.056	-594.492
41	NpO2(CO3)2=- NpO2(CO3)2=-	aqueous	389.065	-808.403
42	NpO2(CO3)3==- NpO2(CO3)3==-	aqueous	449.075	-1019.918
43	Am+++ Am+++	aqueous	243.000	-241.694
44	AmCO3+ AmCO3+	aqueous	303.009	-472.060
45	Am(CO3)2- Am(CO3)2-	aqueous	363.018	-695.880
46	Am(CO3)3=- Am(CO3)3=-	aqueous	423.028	-915.460
47	Am(OH)2+ Am(OH)2+	aqueous	277.015	-393.647
48	Am(OH)3(aq) Am(OH)3(aq)	aqueous	294.022	-462.950
49	Th++++ Th++++	aqueous	232.038	-999.990
50	UO2++ U(VI)O2++	aqueous	270.028	-999.990
51	NpO2OH(aged)_____NpO2OH(aged)	solid	*286.054*	*-454.010*
52	NpO2OH(amor)_____NpO2OH(amor)	solid	286.054	-452.642
53	NaNpO2CO3(s)_____NaNpO2CO3(s)	solid	352.046	-713.707
54	Na3NpO2(CO3)2(s)_DISABLED_DISABLED	solid	458.035	999.990
55	AmOHCO3(c)_____AmOHCO3(c)	solid	320.017	-569.980
56	Am(OH)3(s)_____Am(OH)3(s)	solid	294.022	-492.294
57	NaAm(CO3)2.6H2O(c)_____	solid	494.099	-1396.494
58	AmPO4(c)_____AmPO4(c)	solid	337.972	-709.750
59	CaSO4_____Anhydrite	solid	136.138	-533.730
60	NaK3(SO4)2__Aphthitalite/Glaserite	solid	332.400	-1057.050
61	CaCl2.6H2O_____Antarcticite	solid	219.077	-893.650
62	CaCO3_____Aragonite	solid	100.089	-455.170
63	K2SO4_____Arcanite	solid	174.254	-532.390
64	MgCl2.6H2O_____Bischofite	solid	203.302	-853.100
65	Na2Mg(SO4)2.4H2O_____Bloedite	solid	334.461	-1383.600
66	Mg(OH)2_____Brucite	solid	58.320	-335.400
67	Na6CO3(SO4)2_____Burkeite	solid	390.063	-1449.400
68	CaCO3_____Calcite	solid	100.089	-455.600
69	CaCl2.4H2O_____CaCl2_Tetrahydrite	solid	183.047	-698.700
70	Ca4Cl2(OH)6.13H2O__CaOxychloride A	solid	567.467	-2658.450
71	Ca2Cl2(OH)2.H2O____CaOxychloride B	solid	203.096	-778.410
72	KMgCl3.6H2O_____Carnallite	solid	277.854	-1020.300
73	MgSO4.7H2O_____Epsomite	solid	246.469	-1157.830
74	CaNa2(CO3)2.5H2O_____Gaylussite	solid	296.154	-1360.500
75	Na2Ca(SO4)2_____Glauberite	solid	278.175	-1047.450
76	CaSO4.2H2O_____Gypsum	solid	172.168	-725.560
77	NaCl_____Halite	solid	58.443	-154.990
78	MgSO4.6H2O_____Hexahydrite	solid	228.454	-1061.600
79	*KMgClSO4.3H2O_____Kainite*	*solid*	*248.960*	*-938.200*
80	KHCO3_____Kalicinite	solid	100.115	-350.060
81	MgSO4.H2O_____ Kieserite	solid	138.378	-579.800
82	K2Mg(SO4)2.4H2O_____Leonite	solid	366.678	-1403.970
83	Na4Ca(SO4)3.2H2O_____Labile_Salt	solid	456.242	-1751.450
84	MgCO3_____Magnesite	solid	84.314	-414.450
85	Mg2Cl(OH)3.4H2O_____MgOxychloride	solid	207.146	-1029.600
86	KHSO4_____Mercallite	solid	136.164	-417.570
87	Na2SO4.10H2O_____Mirabilite	solid	322.189	-1471.150
88	K8H6(SO4)7_____Misenite	solid	991.237	-3039.240
89	NaHCO3_____Nahcolite	solid	84.007	-343.330
90	Na2CO3.10H2O_____Natron	solid	286.141	-1382.780
91	MgCO3.3H2O_____Nesquehonite	solid	138.360	-695.300
92	K2Mg(SO4)2.6H2O Picromerite/Schoen	solid	402.708	-1596.100
93	Na2Ca(CO3)2.2H2O_____Pirssonite	solid	242.108	-1073.100
94	K2MgCa2(SO4)4.2H2O_____Polyhalite	solid	602.922	-2282.500
95	Ca(OH)2_____Portlandite	solid	74.095	-362.120
96	K2CO3.3/2H2O___Potassium_Carbonate	solid	165.229	-577.370
97	K8H4(CO3)6.3H2O___K-Sequicarbonate	solid	730.919	-2555.400
98	*KNaCO3.6H2O_____K-Na-Carbonate*	*solid*	*230.188*	*-1006.800*
99	K2NaH(CO3)2.2H2O___Potassium_Trona	solid	258.243	-971.740
100	K3H(SO4)2__Sesquipotassium_Sulfate	solid	310.418	-950.800
101	Na3H(SO4)2____Sesquisodium_Sulfate	solid	262.092	-919.600
102	Na2CO3.7H2O____Na2CO3-Heptahydrate	solid	232.095	-1094.950
103	KCl_____Sylvite	solid	74.551	-164.840
104	K2Ca(SO4)2.H2O_____Syngenite	solid	328.407	-1164.800
105	Mg2CaCl6.12H2O_____Tachyhydrite	solid	517.590	-2015.900
106	Na2SO4_____Thenardite	solid	142.037	-512.350
107	Na2CO3.H2O_____Thermonatrite	solid	124.004	-518.800
108	Na3H(CO3)2.2H2O_____Trona	solid	226.026	-960.380
109	Na2B4O7.10H2O_____ Borax	solid	381.367	-2224.160
110	B(OH)3_____Borix_Acid_Solid	solid	61.832	-390.880
111	KB5O8.4H2O____K-Pentaborate_(30_C)	solid	293.204	-1770.260
112	K2B4O7.4H2O___K-Tetraborate_(30_C)	solid	305.493	-1663.470
113	NaBO2.4H2O_____Sodium_Metaborate	solid	137.859	-761.420
114	NaB5O8.5H2O_____Sodium_Pentaborate	solid	295.111	-1854.800
115	NaBO2.NaCl.2H2O___Teepleite_(20_C)	solid	160.272	-725.770

	Truncated Name	Formula Matrix
1	H2O	2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2	Na+	0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

```
1433    3 K+                          0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
1434    4 Ca++                        0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
1435    5 Mg++                        0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
1436    6 MgOH+                       1  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
1437    7 H+                          1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
1438    8 Cl-                         0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 -1
1439    9 SO4=                        0  4  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 -2
1440   10 HSO4-                       1  4  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 -1
1441   11 OH-                         1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 -1
1442   12 HCO3-                       1  3  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0 -1
1443   13 CO3=                        0  3  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0 -2
1444   14 CO2(aq)                     0  2  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1445   15 CaCO3(aq)                   0  3  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1446   16 MgCO3(aq)                   0  3  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1447   17 B(OH)3(aq)                  3  3  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0
1448   18 B(OH)4-                     4  4  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0 -1
1449   19 B3O3(OH)4-                  4  7  0  0  0  0  0  0  0  0  0  0  3  0  0  0  0  0  0  0  0  0  0 -1
1450   20 B4O5(OH)4=                  4  9  0  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0  0 -2
1451   21 CaB(OH)4+                   4  4  0  0  0  1  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  1
1452   22 MgB(OH)4+                   4  4  0  0  1  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  1
1453   23 Br-                         0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0 -1
1454   24 ClO4-                 pe    0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0 -1
1455   25 NaOH(aq).....to.ti          1  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1456   26 HCl(aq).....to.ti           1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1457   27 HClO4(aq).....to.ti         1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0
1458   28 PosIon.....                 0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  1
1459   29 NegIon.....                 0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0 -1
1460   30 PosIon(OH)(aq).....         1  1  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1461   31 HNegIon(aq).....            1  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
1462   32 Tracer(aq).....cons         0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0
1463   33 H3PO4(aq)                   3  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0
1464   34 H2PO4-                      2  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0 -1
1465   35 HPO4=                       1  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0 -2
1466   36 PO4=-                       0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0 -3
1467   37 NpO2+                       0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  1
1468   38 NpO2OH(aq)                  1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0
1469   39 NpO2(OH)2-                  2  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0 -1
1470   40 NpO2CO3-                    0  5  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  1  0  0 -1
1471   41 NpO2(CO3)2=-                0  8  0  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  1  0  0 -3
1472   42 NpO2(CO3)3==-               0 11  0  0  0  0  0  0  3  0  0  0  0  0  0  0  0  0  0  0  1  0  0 -5
1473   43 Am+++                       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  3
1474   44 AmCO3+                      0  3  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  1  0  0  0  0  1
1475   45 Am(CO3)2-                   0  6  0  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  1  0  0  0  0 -1
1476   46 Am(CO3)3=-                  0  9  0  0  0  0  0  0  3  0  0  0  0  0  0  0  0  0  1  0  0  0  0 -3
1477   47 Am(OH)2+                    2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  1
1478   48 Am(OH)3(aq)                 3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
1479   49 Th++++                      0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  4
1480   50 UO2++                       0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  2
1481   51 NpO2OH(aged)_______         1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0
1482   52 NpO2OH(amor)_______         1  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0
1483   53 NaNpO2CO3(s)_____           0  5  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0
1484   54 Na3NpO2(CO3)2(s)_DI         0  8  3  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0
1485   55 AmOHCO3(c)_____             1  4  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
1486   56 Am(OH)3(s)_____             3  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
1487   57 NaAm(CO3)2.6H2O(c)_        12 12  1  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
1488   58 AmPO4(c)_____               0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  1  0
1489   59 CaSO4_____                  0  4  0  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1490   60 NaK3(SO4)2__Aphthit         0  8  1  3  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1491   61 CaCl2.6H2O_____            12  6  0  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1492   62 CaCO3_____                  0  3  0  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1493   63 K2SO4_____                  0  4  0  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1494   64 MgCl2.6H2O_____            12  6  0  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1495   65 Na2Mg(SO4)2.4H2O___         8 12  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1496   66 Mg(OH)2_____                2  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1497   67 Na6CO3(SO4)2_____           0 11  6  0  0  0  0  0  2  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1498   68 CaCO3_____                  0  3  0  0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1499   69 CaCl2.4H2O_____CaC          8  4  0  0  0  0  1  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1500   70 Ca4Cl2(OH)6.13H2O__        32 19  0  0  0  0  4  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1501   71 Ca2Cl2(OH)2.H2O____         4  3  0  0  0  0  2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1502   72 KMgCl3.6H2O_____           12  6  0  1  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1503   73 MgSO4.7H2O_____            14 11  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1504   74 CaNa2(CO3)2.5H2O___        10 11  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1505   75 Na2Ca(SO4)2_____            0  8  2  0  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1506   76 CaSO4.2H2O_____             4  6  0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1507   77 NaCl_____                   0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1508   78 MgSO4.6H2O_____            12 10  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1509   79 KMgClSO4.3H2O_____          6  7  0  1  1  0  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1510   80 KHCO3_____                  1  3  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1511   81 MgSO4.H2O_____              2  5  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1512   82 K2Mg(SO4)2.4H2O____         8 12  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1513   83 Na4Ca(SO4)3.2H2O___         4 14  4  0  0  1  0  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1514   84 MgCO3_____                  0  3  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1515   85 Mg2Cl(OH)3.4H2O____        11  7  0  0  2  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1516   86 KHSO4_____                  1  4  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1517   87 Na2SO4.10H2O_____          20 14  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1518   88 K8H6(SO4)7_____             6 28  0  8  0  0  0  7  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1519   89 NaHCO3_____                 1  3  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1520   90 Na2CO3.10H2O_____          20 13  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1521   91 MgCO3.3H2O_____             6  6  0  0  1  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1522   92 K2Mg(SO4)2.6H2O Pic        12 14  0  2  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
```

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

```
1523   93 Na2Ca(CO3)2.2H2O___    4  8  2  0  0  1  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1524   94 K2MgCa2(SO4)4.2H2O_    4 18  0  2  1  2  0  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1525   95 Ca(OH)2_____           2  2  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1526   96 K2CO3.3/2H2O___Pota    3  4  0  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1527   97 K8H4(CO3)6.3H2O___K   10 21  0  8  0  0  0  0  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1528   98 KNaCO3.6H2O_____      12  9  1  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1529   99 K2NaH(CO3)2.2H2O___    5  8  1  2  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1530  100 K3H(SO4)2__Sesquipo    1  8  0  3  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1531  101 Na3H(SO4)2____Sesqu    1  8  3  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1532  102 Na2CO3.7H2O____Na2C   14 10  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1533  103 KCl_____              0  0  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1534  104 K2Ca(SO4)2.H2O_____   2  9  0  2  0  1  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1535  105 Mg2CaCl6.12H2O_____  24 12  0  0  2  1  6  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1536  106 Na2SO4_____           0  4  2  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1537  107 Na2CO3.H2O_____       2  4  2  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1538  108 Na3H(CO3)2.2H2O____   5  8  3  0  0  0  0  0  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1539  109 Na2B4O7.10H2O_____   20 17  2  0  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0  0  0
1540  110 B(OH)3_____________B  3  3  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0
1541  111 KB5O8.4H2O____K-Pen   8 12  0  1  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0  0
1542  112 K2B4O7.4H2O___K-Tet   8 11  0  2  0  0  0  0  0  0  0  0  4  0  0  0  0  0  0  0  0  0  0
1543  113 NaBO2.4H2O_____So     8  6  1  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
1544  114 NaB5O8.5H2O_____Sod  10 13  1  0  0  0  0  0  0  0  0  0  5  0  0  0  0  0  0  0  0  0  0
1545  115 NaBO2.NaCl.2H2O___T   4  4  2  0  0  0  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
1546 ********************************************************************************************************
```

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

K.1 Listing

See Table 25 for explanation of this listing.

```
     2.d3   'Np(V)O2OH(aged)....Np(V)O2OH(aged)'
     2.d3   'Np(V)O2OH(amor)....Np(V)O2OH(amor)'
     2.d3   'NaNp(V)O2CO3(s)....NaNp(V)O2CO3(s)'
     2.d3   'NaNpO2CO3Na2CO3(s)Na3NpO2(CO3)2(s)'
     2.d3    AmOHCO3(c)
     2.d3    Am(OH)3(s)
     2.d3    NaAm(CO3)2.6H2O(c)
     2.d3    AmPO4(c)

  2980.d0   CaSO4                    Anhydrite  CRC p.B-181:185
     2.d3   NaK3(SO4)2  Aphthitalite/Glaserite
     2.d3   CaCl2.6H2O             Antarcticite
  2940.d0   CaCO3                     Aragonite  CRC p.B-181:185
  2663.d0   K2SO4                     Arcanite  CRC p.B-181:185
     2.d3   MgCl2.6H2O               Bischofite
  2250.d0   Na2Mg(SO4)2.4H2O           Bloedite  CRC p.B-181:185
  2390.d0   Mg(OH)2                     Brucite  CRC p.B-181:185
     2.d3   Na6CO3(SO4)2               Burkeite
  2828.d0   CaCO3                      Calcite  CRC p.B-181:185
     2.d3   CaCl2.4H2O       CaCl2 Tetrahydrite
     2.d3   Ca4Cl2(OH)6.13H2O  CaOxychloride A
     2.d3   Ca2Cl2(OH)2.H2O    CaOxychloride B
  1602.d0   KMgCl3.6H2O              Carnallite  CRC p.B-181:185
  1677.d0   MgSO4.7H2O                 Epsomite  CRC p.B-181:185
  1991.d0   CaNa2(CO3)2.5H2O         Gaylussite  CRC p.B-181:185
  2800.d0   Na2Ca(SO4)2              Glauberite  CRC p.B-181:185
  2335.d0   CaSO4.2H2O                   Gypsum  CRC p.B-181:185
  2165.d0   NaCl                        Halite  CRC p.B-181:185
     2.d3   MgSO4.6H2O               Hexahydrite
  2150.d0   KMgClSO4.3H2O               Kainite  CRC p.B-181:185
     2.d3   KHCO3                     Kalicinite
  2571.d0   MgSO4.H2O                  Kieserite  CRC p.B-181:185
     2.d3   K2Mg(SO4)2.4H2O              Leonite
     2.d3   Na4Ca(SO4)3.2H2O         Labile Salt
  3210.d0   MgCO3                      Magnesite  CRC p.B-181:185
     2.d3   Mg2Cl(OH)3.4H2O       MgOxychloride
     2.d3   KHSO4                     Mercallite
  1490.d0   Na2SO4.10H2O              Mirabilite  CRC p.B-181:185
     2.d3   K8H6(SO4)7                  Misenite
     2.d3   NaHCO3                     Nahcolite
     2.d3   Na2CO3.10H2O                 Natron
     2.d3   MgCO3.3H2O              Nesquehonite
     2.d3   K2Mg(SO4)2.6H2O Picromerite/Schoen
     2.d3   Na2Ca(CO3)2.2H2O          Pirssonite
     2.d3   K2MgCa2(SO4)4.2H2O        Polyhalite
     2.d3   Ca(OH)2                   Portlandite
     2.d3   K2CO3.3/2H2O   Potassium Carbonate
     2.d3   K8H4(CO3)6.3H2O   K-Sequicarbonate
     2.d3   KNaCO3.6H2O          K-Na-Carbonate
     2.d3   K2NaH(CO3)2.2H2O   Potassium Trona
     2.d3   K3H(SO4)2  Sesquipotassium Sulfate
     2.d3   Na3H(SO4)2    Sesquisodium Sulfate
     2.d3   Na2CO3.7H2O    Na2CO3-Heptahydrate
  1990.d0   KCl                         Sylvite  CRC p.B-181:185
     2.d3   K2Ca(SO4)2.H2O             Syngenite
     2.d3   Mg2CaCl6.12H2O          Tachyhydrite
     2.d3   Na2SO4                     Thenardite
  2255.d0   Na2CO3.H2O             Thermonatrite  CRC p.B-181:185
  2140.d0   Na3H(CO3)2.2H2O                Trona  CRC p.B-181:185
  1715.d0   Na2B4O7.10H2O                  Borax  CRC p.B-181:185
     2.d3   B(OH)3              Borix Acid Solid
     2.d3   KB5O8.4H2O    K-Pentaborate (30 C)
     2.d3   K2B4O7.4H2O   K-Tetraborate (30 C)
     2.d3   NaBO2.4H2O        Sodium Metaborate
     2.d3   NaB5O8.5H2O      Sodium Pentaborate
     2.d3   NaBO2.NaCl.2H2O   Teepleite (20 C)
```

K.2 References Cited in Listing

Novak, C.F. 1994. "Development of the FMT Chemical Transport Simulator: Coupling Aqueous Density and Mineral Volume Fraction to Phase Composition." *Proceedings of the*

Fourth International Conference on the Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere . Special Issue of Radiochimica Acta. R. Oldenbourg Verlag: München, Germany.

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

Appendix L: Output File Listing of HMW_NP_AM.RHOMIN

```
MINERAL DENSITIES, KG/M^3, IN FILE "RHOMIN"

NpO2OH(aged)__________NpO2OH(aged)    2000.00000000000
NpO2OH(amor)__________NpO2OH(amor)    2000.00000000000
NaNpO2CO3(s)__________NaNpO2CO3(s)    2000.00000000000
Na3NpO2(CO3)2(s)_DISABLED_DISABLED    2000.00000000000
AmOHCO3(c)_____________AmOHCO3(c)     2000.00000000000
Am(OH)3(s)_____________Am(OH)3(s)     2000.00000000000
NaAm(CO3)2.6H2O(c)_____________       2000.00000000000
AmPO4(c)_____________AmPO4(c)         2000.00000000000
CaSO4_____________Anhydrite           2980.00000000000
NaK3(SO4)2__Aphthitalite/Glaserite    2000.00000000000
CaCl2.6H2O_____________Antarcticite   2000.00000000000
CaCO3_____________Aragonite           2940.00000000000
K2SO4_____________Arcanite            2663.00000000000
MgCl2.6H2O_____________Bischofite     2000.00000000000
Na2Mg(SO4)2.4H2O_____Bloedite         2250.00000000000
Mg(OH)2_____________Brucite           2390.00000000000
Na6CO3(SO4)2_____________Burkeite     2000.00000000000
CaCO3_____________Calcite             2828.00000000000
CaCl2.4H2O_____CaCl2_Tetrahydrite     2000.00000000000
Ca4Cl2(OH)6.13H2O__CaOxychloride A    2000.00000000000
Ca2Cl2(OH)2.H2O____CaOxychloride B    2000.00000000000
KMgCl3.6H2O_____________Carnallite    1602.00000000000
MgSO4.7H2O_____________Epsomite       1677.00000000000
CaNa2(CO3)2.5H2O_____Gaylussite       1991.00000000000
Na2Ca(SO4)2_____________Glauberite    2800.00000000000
CaSO4.2H2O_____________Gypsum         2335.00000000000
NaCl_____________Halite               2165.00000000000
MgSO4.6H2O_____________Hexahydrite    2000.00000000000
KMgClSO4.3H2O_____________Kainite     2150.00000000000
KHCO3_____________Kalicinite          2000.00000000000
MgSO4.H2O_____________ Kieserite      2571.00000000000
K2Mg(SO4)2.4H2O_____________Leonite   2000.00000000000
Na4Ca(SO4)3.2H2O_____Labile_Salt      2000.00000000000
MgCO3_____________Magnesite           3210.00000000000
Mg2Cl(OH)3.4H2O_____MgOxychloride     2000.00000000000
KHSO4_____________Mercallite          2000.00000000000
Na2SO4.10H2O_____________Mirabilite   1490.00000000000
K8H6(SO4)7_____________Misenite       2000.00000000000
NaHCO3_____________Nahcolite          2000.00000000000
Na2CO3.10H2O_____________Natron       2000.00000000000
MgCO3.3H2O_____________Nesquehonite   2000.00000000000
K2Mg(SO4)2.6H2O Picromerite/Schoen    2000.00000000000
Na2Ca(CO3)2.2H2O_____Pirssonite       2000.00000000000
K2MgCa2(SO4)4.2H2O_____Polyhalite     2000.00000000000
Ca(OH)2_____________Portlandite       2000.00000000000
K2CO3.3/2H2O___Potassium_Carbonate    2000.00000000000
K8H4(CO3)6.3H2O___K-Sequicarbonate    2000.00000000000
KNaCO3.6H2O_____K-Na-Carbonate        2000.00000000000
K2NaH(CO3)2.2H2O___Potassium_Trona    2000.00000000000
K3H(SO4)2__Sesquipotassium_Sulfate    2000.00000000000
Na3H(SO4)2____Sesquisodium_Sulfate    2000.00000000000
Na2CO3.7H2O____Na2CO3-Heptahydrate    2000.00000000000
KCl_____________Sylvite               1990.00000000000
K2Ca(SO4)2.H2O_____Syngenite          2000.00000000000
Mg2CaCl6.12H2O_____Tachyhydrite       2000.00000000000
Na2SO4_____________Thenardite         2000.00000000000
Na2CO3.H2O_____Thermonatrite          2255.00000000000
Na3H(CO3)2.2H2O_____Trona             2140.00000000000
Na2B4O7.10H2O_____ Borax              1715.00000000000
B(OH)3_____Borix_Acid_Solid           2000.00000000000
KB5O8.4H2O____K-Pentaborate_(30_C)    2000.00000000000
K2B4O7.4H2O___K-Tetraborate_(30_C)    2000.00000000000
NaBO2.4H2O_____Sodium_Metaborate      2000.00000000000
NaB5O8.5H2O_____Sodium_Pentaborate    2000.00000000000
NaBO2.NaCl.2H2O___Teepleite_(20_C)    2000.00000000000
```

Appendix M: Sample Output File "BATCH_DOC.OUT"

See Table 26 for explanation of this listing.

```
 INPUT    file name is U1:[SCBABB.FMT.USERGUIDE]BATCH_DOC.IN;1
 INGUESS  file name is U1:[SCBABB.FMT.USERGUIDE]BATCH_DOC.INGUESS;1
 OUTPUT   file name is U1:[SCBABB.FMT.USERGUIDE]BATCH_DOC.OUT;1
 CHEMDAT  file name is U1:[SCBABB.FMT.USERGUIDE]FMT_HMW_NP_AM.CHEMDAT;1
 Temperature is Hard Coded as 298.15K
 [.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs                FMT V2.0
 DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,F91,RFFR92,RFF94,RRFF94)


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


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

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

          2 Solubility Product Violations
 Adding solid Mg(OH)2____________________Brucite
 # inversions for batch pblm          85
1[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs               FMT V2.0
 DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,F91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

 Elemental Abundances for Flash Problem

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

 Using NaCl Density Correlation
   1.10222364E+02   1.11116160E+02   1.10794086E+02   1.11669359E+05  Hydrogen
   5.51654821E+01   5.56118135E+01   5.54506206E+01   8.87176559E+05  Oxygen
   2.00000000E-01   2.01625464E-01   2.01041045E-01   4.62188739E+03  Sodium
   1.00000000E-02   1.00812732E-02   1.00520523E-02   3.93018155E+02  Potassium
   1.00000000E-03   4.64673729E-08   4.63326856E-08   1.12611592E-03  Magnesium
   1.00000000E-04   1.00812732E-04   1.00520523E-04   4.02886254E+00  Calcium
   1.10000000E-01   1.10894005E-01   1.10572575E-01   3.92012950E+03  Chlorine
   1.00000000E-03   1.00812732E-03   1.00520523E-03   3.22268795E+01  Sulfur
   1.00000000E-04   1.00812732E-04   1.00520523E-04   1.20735200E+00  Carbon
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
   1.00000000E-07   1.00812732E-07   1.00520523E-07   1.08662685E-03  Boron
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Np(V)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
   4.90605392E-17   4.94592698E-17   4.93159103E-17   0.00000000E+00  Charge

   Solution Parameters, Calculated
     SOLUTION MASS     1002.59976105542      grams
     H2O MASS          991.93820129674D      grams
     TDS(g/kg)         10.7482096613917      g/kgH2O

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

   Solution Parameters Based on Specified Density
     SOLUTION VOL    0.994821728428285       liters
     TDS               10.7170555829388      g/l

   Density based on TDS and NaCl solutions    1007.81851904202      g/l
   Percent relative error vs NaCl density    0.0000000000000000E+000 %


 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

 H2O                        WATER      9.92444E-01   9.93023E-01    1.001        5.50612E+01   5.53478E+01   9.97101E+05
 Na+                          Na+      2.01625E-01   1.47085E-01   0.7295        2.00000E-01   2.01041E-01   4.62189E+03
```

Appendix M: Sample Output File "BATCH_DOC.OUT"

83	Cl-	Cl-	1.10894E-01	7.98916E-02	0.7204	1.10000E-01	1.10573E-01	3.92013E+03	
84	OH-	OH-	9.87965E-02	7.13753E-02	0.7224	9.80001E-02	9.85102E-02	1.67539E+03	
85	K+	K+	1.00813E-02	7.34149E-03	0.7282	1.00000E-02	1.00521E-02	3.93018E+02	
86	SO4=	SO4=	1.00813E-03	2.24998E-04	0.2232	1.00000E-03	1.00521E-03	9.65576E+01	
87	Mg(OH)2	Brucite	1.00808E-03	1.00000E+00	1.000	9.99954E-04	1.00516E-03	5.86205E+01	
88	Ca++	Ca++	1.00115E-04	2.00966E-05	0.2007	9.93083E-05	9.98252E-05	4.00099E+00	
89	CO3=	CO3=	1.00005E-04	2.44915E-05	0.2449	9.91991E-05	9.97155E-05	5.98385E+00	
90	B(OH)4-	B(OH)4-	1.00709E-07	6.61270E-08	0.6566	9.98971E-08	1.00417E-07	7.91680E-03	
91	CaCO3(aq)	CaCO3(aq)	6.97236E-07	6.97236E-07	1.000	6.91615E-07	6.95215E-07	6.95835E-02	1.38E-10
92	HCO3-	HCO3-	1.10094E-07	7.49923E-08	0.6812	1.09206E-07	1.09775E-07	6.69815E-03	1.60E-10
93	MgOH+	MgOH+	3.54268E-08	2.81647E-08	0.7950	3.51412E-08	3.53241E-08	1.45932E-03	-2.47E-07
94	Mg++	Mg++	1.09873E-08	2.56221E-09	0.2332	1.08988E-08	1.09555E-08	2.66273E-04	2.36E-10
95	CaB(OH)4+	CaB(OH)4+	8.72370E-11	5.94047E-11	0.6810	8.65337E-11	8.69841E-11	1.03441E-05	3.87E-11
96	MgCO3(aq)	MgCO3(aq)	5.32206E-11	5.32206E-11	1.000	5.27915E-11	5.30663E-11	4.47424E-06	3.15E-10
97	B(OH)3(aq)	B(OH)3(aq)	1.65411E-11	1.61858E-11	0.9785	1.64077E-11	1.64931E-11	1.01980E-06	1.62E-10
98	H+	H+	1.93212E-13	1.40201E-13	0.7256	1.91654E-13	1.92652E-13	1.94173E-10	1.36E-10
99	CO2(aq)	CO2(aq)	2.21142E-14	2.30277E-14	1.041	2.19360E-14	2.20501E-14	9.70422E-10	3.16E-10
100	MgB(OH)4+	MgB(OH)4+	6.18470E-15	4.24905E-15	0.6870	6.13484E-15	6.16677E-15	6.36066E-10	2.98E-10
101	HSO4-	HSO4-	4.06799E-15	3.00314E-15	0.7382	4.03519E-15	4.05620E-15	3.93717E-10	2.03E-10
102	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
103	K8H6(SO4)7	Misenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+02
104	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
105	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
106	B(OH)3	Borix_Acid_Solid	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.08E+01
107	Na2B4O7.10H2O	Borax	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.16E+01
108	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
109	Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.76E+00
110	Na2SO4	Thenardite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.03E+00
111	Mg2CaCl6.12H2O	Tachyhydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.59E+01
112	K2Ca(SO4)2.H2O	Syngenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.82E+00
113	KCl	Sylvite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.13E+00
114	Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.84E+00
115	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
116	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
117	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
118	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
119	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
120	Ca(OH)2	Portlandite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.80E+00
121	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
122	Na2Ca(CO3)2.2H2O	Pirssonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.35E+00
123	K2Mg(SO4)2.6H2O	Picromerite/Schoen	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.58E+01
124	MgCO3.3H2O	Nesquehonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.04E+00
125	Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.48E+00
126	NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.55E+00
127	NaBO2.4H2O	Sodium_Metaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.35E+00
128	Na2SO4.10H2O	Mirabilite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.12E+00
129	KHSO4	Mercallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.72E+01
130	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
131	MgCO3	Magnesite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.37E+00
132	Na4Ca(SO4)3.2H2O	Labile_Salt	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.33E+01
133	K2Mg(SO4)2.4H2O	Leonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+01
134	MgSO4.H2O	Kieserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.21E+01
135	KHCO3	Kalicinite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.54E+00
136	KMgClSO4.3H2O	Kainite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.53E+01
137	MgSO4.6H2O	Hexahydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.06E+01
138	NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.50E+00
139	CaSO4.2H2O	Gypsum	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.77E+00
140	Na2Ca(SO4)2	Glauberite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.41E+00
141	CaNa2(CO3)2.5H2O	Gaylussite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.18E+00
142	MgSO4.7H2O	Epsomite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.04E+01
143	KMgCl3.6H2O	Carnallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.84E+01
144	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
145	CaCl2.4H2O	CaCl2_Tetrahydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.26E+01
146	CaCO3	Calcite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.02E-01
147	Na6CO3(SO4)2	Burkeite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.61E+01
148	Na2Mg(SO4)2.4H2O	Bloedite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.52E+01
149	MgCl2.6H2O	Bischofite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.53E+01
150	K2SO4	Arcanite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.14E+00
151	CaCO3	Aragonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+00
152	CaCl2.6H2O	Antarcticite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.11E+01
153	NaK3(SO4)2	Aphthitalite/Glaserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.07E+01
154	CaSO4	Anhydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.98E+00
155	NaBO2.NaCl.2H2O	Teepleite_(20_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.15E+01
156	NaB5O8.5H2O	Sodium_Pentaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.78E+01
157	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
158	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
159	B4O5(OH)4=	B4O5(OH)4=	0.00000E+00	0.00000E+00	0.1519	0.00000E+00	0.00000E+00	0.00000E+00	-3.36E+01
160	K8H4(CO3)6.3H2O	K-Sequicarbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.18E+01
161	B3O3(OH)4-	B3O3(OH)4-	0.00000E+00	0.00000E+00	0.5412	0.00000E+00	0.00000E+00	0.00000E+00	-2.70E+01

162

163 pmH = -log[m(H+)] = 12.7140

164 pH = -log[a(H+)] = 12.8532

165 Osmotic Coefficient= 0.919612

166 Equilibrium RH (%) = 99.302313

167 Ionic Strength (m) = 0.213115

168 Density, kg/m3 = 1007.82

169

170 NOTES: - Water "molality" is mole fraction H2O in aqueous phase

171 - Gas "molality" and "activity" are gas partial pressures

172 - "Descriptor" means:

```
          *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
          *Saturation Index for minerals, SI=log10(IAP/Ksp)
          *log10(activity) for aqueous species with very small concentrations
          *log10(partial pressure) for gases

Total G/RT=     -5.30370149E+03

Total Diagonal Inversions           85
Total Stoichiometric Reoptimizations           10
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

See Table 27 for explanation of this listing.

```
 1  INPUT    file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LOG.IN;1
 2  INGUESS  file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LOG.INGUESS;1
 3  OUTPUT   file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LOG.OUT;1
 4  CHEMDAT  file name is U1:[SCBABB.FMT.USERGUIDE]FMT_HMW_NP_AM.CHEMDAT;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 V2.0
 7  DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 8  95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
 9
10
11  ********************************************************************************************************************************************
12  *** ECHO PRINT OF "CHEMDAT" FILE WOULD BE HERE ***
13  ***               SEE APPENDIX J                ***
14  ********************************************************************************************************************************************
15
16
17  TITRATION Problem:
18   -) Assigning all delta(y) to 0.1 m
19   -) Setting # of nodes in Y-direction to 3
20   -) Setting NONREACTIVE Porosity to 0.0
21
22
23
24  Specifying VARIABLE POROSITY for TITRATION Problem
25
26
27  Aqueous Density is a Function of Composition
28
29  RHOMIN   file name is U1:[SCBABB.FMT.USERGUIDE]FMT_HMW_NP_AM.RHOMIN;1
30
31  ********************************************************************************************************************************************
32  *** TABLE OF MINERAL DENSITIES, KG/M^3 WOULD BE HERE ***
33  ***                SEE APPENDIX L                    ***
34  ********************************************************************************************************************************************
35
36  GRID BLOCK VOLUMES, in liters
37   1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
38   1.00E+00  1.00E+00
39
40   1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
41   1.00E+00  1.00E+00
42
43   1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
44   1.00E+00  1.00E+00
45
46  # inversions for batch pblm           50
47 1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
48  DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
49  95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
50      Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin
51
52  Elemental Abundances for Flash Problem
53
54    Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
55
56    1.11017363E+02   1.11029658E+02   1.00100314E+02   1.00891107E+05  Hydrogen
57    6.15086815E+01   6.15154934E+01   5.54601388E+01   8.87328944E+05  Oxygen
58    5.61000000E+00   5.61062129E+00   5.05833276E+00   1.16289907E+05  Sodium
59    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
60    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
61    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
62    1.61000000E+00   1.61017830E+00   1.45167838E+00   5.14663538E+04  Chlorine
63    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
64    2.00000001E+00   2.00022150E+00   1.80332719E+00   2.16597629E+04  Carbon
65    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
66    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
67    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
68    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
69    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
70    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
71    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
72    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
73    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
74    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Np(V)
75    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
76    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
77    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
78   -2.22044605E-15  -2.22069196E-15  -2.00209536E-15   0.00000000E+00  Charge
79
80    Solution Parameters, Calculated
81      SOLUTION MASS     1306.07033909890      grams
82      H2O MASS          999.889265717486      grams
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
    TDS(g/kg)          306.214981877726       g/kgH2O

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

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

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



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                              Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                              WATER    8.57464E-01   8.59843E-01    1.003        5.55025E+01   5.00446E+01   9.01564E+05
Na+                                Na+    5.61062E+00   3.69881E+00    0.6593       5.61000E+00   5.05833E+00   1.16290E+05
CO3=                              CO3=    1.99407E+00   4.09214E-02   2.0522E-02    1.99385E+00   1.79778E+00   1.07884E+05
Cl-                                Cl-    1.61018E+00   1.06477E+00    0.6613       1.61000E+00   1.45168E+00   5.14664E+04
HCO3-                            HCO3-    6.14734E-03   1.59044E-03    0.2587       6.14666E-03   5.54222E-03   3.38170E+02
OH-                                OH-    6.14733E-03   4.86901E-03    0.7921       6.14665E-03   5.54221E-03   9.42580E+01    2.00E-11
CO2(aq)                        CO2(aq)    2.36876E-09   7.15913E-09    3.022        2.36850E-09   2.13559E-09   9.39868E-05   -2.12E-07
H+                                  H+    2.39954E-12   1.77959E-12    0.7416       2.39927E-12   2.16334E-12   2.18043E-09   -8.58E-08
Na3H(CO3)2.2H2O_____________Trona      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.57E+00
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
NaCl_____________________________Halite      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -9.75E-01
NaHCO3_____________________Nahcolite      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.83E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.51E-01
Na2CO3.H2O_____________Thermonatrite      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.99E-01
Na2CO3.10H2O_____________Natron      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -8.30E-02

pmH = -log[m(H+)}                 =     11.6199
pH = -log[a(H+)]     =     11.7497
Osmotic Coefficient=     0.908418
Equilibrium RH (%) =    85.9842B4
Ionic Strength (m) =     7.604695
Density, kg/m3     =     1177.64

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

Total G/RT=     -6.42133776E+03

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

shifting left by     4.64434654478256
calling makenuv for allomorphic reactions
# inversions for batch pblm           75
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  1.11018363E+02   1.11017591E+02   9.93838868E+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   5.02297975E+00   1.78079701E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  1.00000000E+01   6.12839261E-04   5.48618892E-04   6.58946152E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  1.00000000E+01   6.12839261E-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
 -2.37316632E-15  -2.37314981E-15  -2.12446380E-15   0.00000000E+00  Charge
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  Solution Parameters, Calculated
    SOLUTION MASS     1328.11614865142      grams
    H2O MASS          1000.00695466819      grams
    TDS(g/kg)         328.106912108529      g/kgH2O

  Specified Solution Density
    DENSITY           1188.93254605477      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL      1.11706602116201      liters
    TDS               293.724084134187      g/l

  Density based on TDS and NaCl solutions    1188.93254605477      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                          WATER    8.31822E-01   7.77959E-01   0.9352        5.55091E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)         9.99932E+00   1.00000E+00    1.000        9.99939E+00   8.95147E+00   3.15133E+06
Cl-                            Cl-    5.61096E+00   5.29329E+00   0.9434        5.61100E+00   5.02298E+00   1.78080E+05
Na+                            Na+    5.61057E+00   5.29268E+00   0.9433        5.61061E+00   5.02263E+00   1.15469E+05
NpO2+                        NpO2+    6.12705E-04   1.21978E-03    1.991        6.12709E-04   5.48499E-04   1.47572E+02
CO2(aq)                    CO2(aq)    3.86103E-04   1.12115E-03    2.904        3.86106E-04   3.45643E-04   1.52117E+01
HCO3-                        HCO3-    2.26571E-04   8.38810E-05   0.3702        2.26573E-04   2.02829E-04   1.23760E+01    4.26E-09
NpO2CO3-                  NpO2CO3-    1.33526E-07   2.42971E-07    1.820        1.33527E-07   1.19534E-07   3.93334E-02   -1.99E-11
H+                              H+    1.21872E-06   4.78095E-06    3.923        1.21873E-06   1.09101E-06   1.09962E-03   -4.38E-08
CO3=                          CO3=    3.09384E-08   8.03342E-10   2.5966E-02    3.09386E-08   2.76963E-08   1.66203E-03   -1.62E-07
OH-                            OH-    3.01685E-09   1.63977E-09   0.5435        3.01687E-09   2.70071E-09   4.59318E-05    2.55E-08
NpO2OH(aq)                NpO2OH(aq)    7.72186E-10   7.72186E-10    1.000        7.72191E-10   6.91267E-10   1.97740E-04    1.87E-07
NpO2(CO3)2=-            NpO2(CO3)2=-    1.98384E-11   5.13354E-16   2.5877E-05    1.98385E-11   1.77595E-11   6.90960E-06   -1.62E-07
NpO2(OH)2-                NpO2(OH)2-    2.04382E-16   6.10703E-17   0.2988        2.04383E-16   1.82964E-16   5.54494E-11    2.13E-07
NpO2(CO3)3==-          NpO2(CO3)3==-    1.25197E-16   9.87896E-26   7.8908E-10    1.25198E-16   1.12077E-16   5.03310E-11   -3.23E-07
NpO2OH(aged)_____NpO2OH(aged)           0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
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
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
Na3NpO2(CO3)2(s)_DISABLED_DISABLED      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NaCl_____________________Halite         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3___________________Nahcolite      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
Na2CO3.10H2O_____________Natron         0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.H2O_____Thermonatrite            0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na3H(CO3)2.2H2O__________Trona          0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
NpO2OH(amor)_____NpO2OH(amor)           0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00

pmH = -log[m(H+)]                 =       5.9141
pH = -log[a(H+)]     =       5.3205
Osmotic Coefficient=     1.241871
Equilibrium RH (%) =    77.795863
Ionic Strength (m) =     5.611188
Density, kg/m3     =      1188.93

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

Total G/RT=     -1.33323084E+04
Flashing Titration #            1
# inversions for batch pblm           11
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.85857174E+01   1.11017591E+02   9.93838868E+01   1.00169020E+05  Hydrogen
  3.66707638E+01   5.55113597E+01   4.96942389E+01   7.95078006E+05  Oxygen
  5.42543623E+00   5.61057382E+00   5.02263316E+00   1.15469181E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95016801E+00   5.61096098E+00   5.02297975E+00   1.78079701E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47561578E+00   6.12839260E-04   5.48618892E-04   6.58946151E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   6.12839260E-04   5.48618892E-04   1.30049121E+02  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -6.94525850E-16  -1.99826754E-15  -1.78886601E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     461.602144251012      grams
    H2O MASS          347.563995068956      grams
    TDS(g/kg)         328.106912108175      g/kgH2O

  Specified Solution Density
    DENSITY           1188.93254605459      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388249228926247       liters
    TDS             293.724084133903        g/l

  Density based on TDS and NaCl solutions    1188.93254605459      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                                WATER  8.31822E-01   7.77959E-01   0.9352        1.92928E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)    9.99932E+00   1.00000E+00   1.000         3.47540E+00   8.95147E+00   3.15133E+06
Cl-                                Cl-    5.61096E+00   5.29329E+00   0.9434        1.95017E+00   5.02298E+00   1.78080E+05
Na+                                Na+    5.61057E+00   5.29268E+00   0.9433        1.95003E+00   5.02263E+00   1.15469E+05
NpO2+                            NpO2+    6.12705E-04   1.21978E-03   1.991         2.12954E-04   5.48499E-04   1.47572E+02
CO2(aq)                        CO2(aq)    3.86103E-04   1.12115E-03   2.904         1.34196E-04   3.45643E-04   1.52117E+01
HCO3-                            HCO3-    2.26571E-04   8.38810E-05   0.3702        7.87481E-05   2.02829E-04   1.23760E+01   -6.17E-15
H+                                  H+    1.21872E-06   4.78095E-06   3.923         4.23582E-07   1.09101E-06   1.09962E-03    6.17E-15
NpO2CO3-                      NpO2CO3-    1.33526E-07   2.42971E-07   1.820         4.64090E-08   1.19534E-07   3.93334E-02    1.85E-14
CO3=                              CO3=    3.09384E-08   8.03343E-10   2.5966E-02    1.07531E-08   2.76963E-08   1.66203E-03    0.00E+00
OH-                                OH-    3.01685E-09   1.63977E-09   0.5435        1.04855E-09   2.70071E-09   4.59318E-05   -6.17E-15
NpO2OH(aq)                  NpO2OH(aq)    7.72186E-10   7.72186E-10   1.000         2.68384E-10   6.91267E-10   1.97740E-04    0.00E+00
NpO2(CO3)2=-              NpO2(CO3)2=-    1.98384E-11   5.13355E-16   2.5877E-05    6.89511E-12   1.77595E-11   6.90960E-06    0.00E+00
NpO2(OH)2-                NpO2(OH)2-      2.04381E-16   6.10703E-17   0.2988        7.10356E-17   1.82964E-16   5.54494E-11    1.23E-14
NpO2(CO3)3==-          NpO2(CO3)3==-      1.25197E-16   9.87897E-26   7.8908E-10    4.35139E-17   1.12077E-16   5.03310E-11   -3.53E-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
NpO2OH(aged)_____________NpO2OH(aged)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
NpO2OH(amor)_____________NpO2OH(amor)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
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
Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NaCl_____________________________Halite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3___________________________Nahcolite 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
Na2CO3.10H2O_____________________Natron   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.H2O_____________Thermonatrite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na3H(CO3)2.2H2O_____________Trona         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01

pmH = -log[m(H+)]                  =      5.9141
pH = -log(a(H+))     =      5.3205
Osmotic Coefficient=     1.241871
Equilibrium RH (%) =    77.795863
Ionic Strength (m) =     5.611188
Density, kg/m3     =      1188.93

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

Total G/RT=     -4.63379813E+03
Flashing Titration #            2
# inversions for batch pblm           13
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM     Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.85957275E+01   1.11017746E+02   9.93891116E+01   1.00174286E+05  Hydrogen
  3.66763098E+01   5.55107903E+01   4.96962723E+01   7.95110540E+05  Oxygen
  5.42594206E+00   5.61014105E+00   5.02250276E+00   1.15466183E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95031318E+00   5.60993114E+00   5.02231483E+00   1.78056128E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47579611E+00   6.90932337E-04   6.18560128E-04   7.42952570E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   1.72218651E-04   1.54179484E-04   3.65479691E+01  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -7.46806759E-16  -2.14813422E-15  -1.92312635E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS     461.665999617224      grams
   H2O MASS          347.653675849716      grams
   TDS(g/kg)         327.947988724253      g/kgH2O

 Specified Solution Density
   DENSITY           1188.85111378691      kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL    0.388329534508870       liters
   TDS               293.596838859300      g/l

 Density based on TDS and NaCl solutions    1188.85111378691      g/l
 Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                                WATER      8.31845E-01   7.78011E-01   0.9353        1.92978E+01   4.96944E+01   8.95254E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)                 9.99718E+00   1.00000E+00   1.000         3.47556E+00   8.95002E+00   3.15082E+06
Na+                                Na+        5.61014E+00   5.29140E+00   0.9432        1.95039E+00   5.02250E+00   1.15466E+05
Cl-                                Cl-        5.60993E+00   5.29139E+00   0.9432        1.95031E+00   5.02231E+00   1.78056E+05
HCO3-                              HCO3-      3.82212E-04   1.41513E-04   0.3702        1.32878E-04   3.42177E-04   2.08787E+01
CO2(aq)                            CO2(aq)    3.08476E-04   8.95671E-04   2.904         1.07243E-04   2.76165E-04   1.21539E+01
NpO2+                              NpO2+      1.72085E-04   3.42481E-04   1.990         5.98258E-05   1.54059E-04   4.14492E+01   -1.64E-12
H+                                 H+         5.77346E-07   2.26410E-06   3.922         2.00716E-07   5.16872E-07   5.20955E-04   -1.59E-11
NpO2CO3-                           NpO2CO3-   1.33573E-07   2.43030E-07   1.819         4.64370E-08   1.19581E-07   3.93490E-02   -2.47E-14
CO3=                               CO3=       1.10196E-07   2.86188E-09   2.5971E-02    3.83099E-08   9.86531E-08   5.92010E-03   2.55E-11
OH-                                OH-        6.37D29E-09   3.46282E-09   0.5436        2.21466E-09   5.70303E-09   9.69932E-05   1.64E-11
NpO2OH(aq)                         NpO2OH(aq) 4.57851E-10   4.57851E-10   1.000         1.59174E-10   4.09893E-10   1.17252E-04   -1.01E-11
NpO2(CO3)2=-                       NpO2(CO3)2=- 7.06677E-11 1.82925E-15   2.5885E-05     2.45679E-11   6.32656E-11   2.46144E-05   2.65E-11
NpO2(CO3)3===-                     NpO2(CO3)3=== 1.58546E-15 1.25406E-24  7.9097E-10     5.51192E-16   1.41939E-15   6.37413E-10   -8.77E-11
NpO2(OH)2-                         NpO2(OH)2- 2.55903E-16   7.64679E-17   0.2988        8.89657E-17   2.29098E-16   6.94309E-11   6.38E-12
Na3H(CO3)2.2H2O_____Trona                     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.40E+00
Na2CO3.H2O_____Thermonatrite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.69E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.40E+00
Na2CO3.10H2O_____Natron                       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.36E+00
NaHCO3_____Nahcolite                          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.72E+00
NaCl_____Halite                               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
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)_____NpO2OH(amor)                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.21E+00
NpO2OH(aged)_____NpO2OH(aged)                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.61E+00
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

 pmH = -log[m(H+)]                 =      6.2386
 pH = -log[a(H+)]     =      5.6451
 Osmotic Coefficient=     1.241740
 Equilibrium RH (%) =    77.801108
 Ionic Strength (m) =     5.610314
 Density, kg/m3     =     1188.85

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

 Total G/RT=     -4.63438031E+03
 Flashing Titration #            3
 # inversions for batch pblm           22
 1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.6lmolal NaCl   FMT V2.0
 DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,F91,RFFR92,RFF94,RRFP94)
      Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
Elemental Abundances for Flash Problem

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

  3.85999827E+01   1.11017943E+02   9.93906557E+01   1.00175842E+05  Hydrogen
  3.66786675E+01   5.55109442E+01   4.96970938E+01   7.95123682E+05  Oxygen
  5.42615710E+00   5.61002979E+00   5.02247225E+00   1.15465482E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95037489E+00   5.60950015E+00   5.02199808E+00   1.78044898E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47587277E+00   7.90126088E-04   7.07373490E-04   8.49626299E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   5.09860080E-05   4.56460697E-05   1.08203186E+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
 -1.85281271E-15  -5.32890020E-15  -4.77078632E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      461.701224245777      grams
    H2O MASS           347.691387660720      grams
    TDS(g/kg)          327.905264930832      g/kgH2O

  Specified Solution Density
    DENSITY            1188.82922071361      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL     0.388366315532383       liters
    TDS              293.562628954494        g/l

  Density based on TDS and NaCl solutions    1188.82922071361      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                              WATER    8.31852E-01   7.78030E-01   0.9353        1.92999E+01   4.96951E+01   8.95267E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)             9.99622E+00   1.00000E+00   1.000         3.47560E+00   8.94928E+00   3.15056E+06
Na+                               Na+     5.61003E+00   5.29080E+00   0.9431        1.95056E+00   5.02247E+00   1.15465E+05
Cl-                               Cl-     5.60950E+00   5.29073E+00   0.9432        1.95037E+00   5.02200E+00   1.78045E+05
HCO3-                             HCO3-   5.79856E-04   2.14695E-04   0.3703        2.01611E-04   5.19125E-04   3.16755E+01
CO2(aq)                           CO2(aq) 2.09763E-04   6.09044E-04   2.903         7.29329E-05   1.87794E-04   8.26478E+00
NpO2+                             NpO2+   5.08519E-05   1.01191E-04   1.990         1.76809E-05   4.55260E-05   1.22486E+01   -9.95E-12
CO3=                              CO3=    3.72979E-07   9.68710E-09   2.5972E-02    1.29682E-07   3.33916E-07   2.00380E-02   -1.22E-10
H+                                H+      2.58813E-07   1.01480E-06   3.921         8.99871E-08   2.31707E-07   2.33537E-04    8.21E-11
NpO2CO3-                          NpO2CO3-  1.33591E-07   2.43057E-07   1.819       4.64484E-08   1.19600E-07   3.93550E-02   -1.23E-14
OH-                               OH-     1.42123E-08   7.72603E-09   0.5436        4.94149E-09   1.27238E-08   2.16397E-04   -8.04E-11
NpO2(CO3)2=-                      NpO2(CO3)2=-  2.39201E-10  6.19248E-15  2.5888E-05  8.31683E-11  2.14149E-10  8.33180E-05  -1.14E-10
NpO2OH(aq)                        NpO2OH(aq)  3.01826E-10  3.01826E-10  1.000       1.04942E-10   2.70215E-10   7.72962E-05    3.40E-11
NpO2(CO3)3=--                     NpO2(CO3)3=--  1.81540E-14  1.43698E-23  7.9155E-10  6.31199E-15  1.62527E-14  7.29866E-09  -3.65E-07
NpO2(OH)2-                        NpO2(OH)2-  3.76383E-16  1.12471E-16  0.2988       1.30865E-16  3.36963E-16  1.02121E-10  -4.63E-11
Na3H(CO3)2.2H2O_____Trona                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.68E+00
Na2CO3.H2O_____Thermonatrite              0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.16E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -6.87E+00
Na2CO3.10H2O_____Natron                   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -6.83E+00
NaHCO3_____Nahcolite                      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.54E+00
NaCl_____Halite                           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.35E+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)_____NpO2OH(amor)             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.39E+00
NpO2OH(aged)_____NpO2OH(aged)             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.79E+00
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

pmH = -log[m(H+)]                 =      6.5870
pH = -log[a(H+)]     =      5.9936
Osmotic Coefficient=     1.241681
Equilibrium RH (%) =    77.803013
Ionic Strength (m) =     5.610081
Density, kg/m3     =     1188.83

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

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
Total G/RT=     -4.63462770E+03
Flashing Titration #            4
# inversions for batch pblm            14
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.86060470E+01   1.11018357E+02   9.93915462E+01   1.00176739E+05  Hydrogen
  3.66820273E+01   5.55118409E+01   4.96981566E+01   7.95140687E+05  Oxygen
  5.42646354E+00   5.61000023E+00   5.02247206E+00   1.15465478E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95046284E+00   5.60889282E+00   5.02148063E+00   1.78026553E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47598202E+00   1.05369370E-03   9.43341702E-04   1.13304772E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   5.04731450E-07   4.51871569E-07   1.07115342E-01  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -8.05334972E-16  -2.31587983E-15  -2.07334069E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     461.766388131816      grams
    H2O MASS          347.744715353115      grams
    TDS(g/kg)         327.889016696973      g/kgH2O

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

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388423849459858       liters
    TDS               293.549618380179      g/l

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


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                              WATER    8.31857E-01   7.78050E-01   0.9353        1.93029E+01   4.96953E+01   8.95271E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)    9.99473E+00   1.00000E+00   1.000         3.47562E+00   8.94800E+00   3.15011E+06
Na+                               Na+    5.61000E+00   5.29000E+00   0.9430        1.95085E+00   5.02247E+00   1.15465E+05
Cl-                               Cl-    5.60889E+00   5.28999E+00   0.9431        1.95046E+00   5.02148E+00   1.78027E+05
HCO3-                           HCO3-    9.92660E-04   3.67543E-04   0.3703        3.45192E-04   8.88700E-04   5.42259E+01
CO3=                             CO3=    5.67888E-05   1.47494E-06   2.5972E-02    1.97480E-05   5.08414E-05   3.05095E+00
CO2(aq)                       CO2(aq)    4.03745E-06   1.17227E-05   2.903         1.40400E-06   3.61461E-06   1.59078E-01   -4.23E-08
OH-                               OH-    1.26397E-06   6.87170E-07   0.5437        4.39540E-07   1.13160E-06   1.92454E-02   -9.18E-08
NpO2+                           NpO2+    3.34101E-07   6.64703E-07   1.990         1.16182E-07   2.99111E-07   8.04750E-02    1.79E-07
NpO2CO3-                     NpO2CO3-    1.33613E-07   2.43094E-07   1.819         4.64631E-08   1.19620E-07   3.93616E-02    3.21E-13
NpO2(CO3)2=-              NpO2(CO3)2=-    3.64205E-08   9.43001E-13   2.5892E-05    1.26650E-08   3.26062E-08   1.26859E-02   -1.15E-07
H+                                 H+    2.91065E-09   1.14100E-08   3.920         1.01216E-09   2.60582E-09   2.62641E-06    1.26E-07
NpO2(CO3)3==-             NpO2(CO3)3=-    4.20660E-10   3.33181E-19   7.9204E-10    1.46282E-10   3.76605E-10   1.69124E-04   -2.16E-07
NpO2OH(aq)                 NpO2OH(aq)    1.76339E-10   1.76339E-10   1.000         6.13211E-11   1.57872E-10   4.51598E-05   -2.06E-08
NpO2(OH)2-                 NpO2(OH)2-    1.95583E-14   5.84438E-15   0.2988        6.80128E-15   1.75100E-14   5.30660E-09   -1.50E-07
Na3H(CO3)2.2H2O_____________Trona      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -6.27E+00
Na2CO3.H2O___________Thermonatrite     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.98E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.69E+00
Na2CO3.10H2O_____________Natron        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.65E+00
NaHCO3_____________________Nahcolite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.31E+00
NaCl_______________________Halite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.33E+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(amor)_____________NpO2OH(amor)  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.62E+00
NpO2OH(aged)_____________NpO2OH(aged)  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.03E+00
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

pmH = -log[m(H+)]                =      8.5360
pH = -log[a(H+)]     =      7.9427
Osmotic Coefficient=     1.241601
Equilibrium RH (%) =    77.805007
Ionic Strength (m) =     5.610057
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
Density, kg/m3      =      1188.82

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

Total G/RT=     -4.63497997E+03
Flashing Titration #            5
# inversions for batch pblm          16
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFP94,RRFF94)
    Pressure=      1.00000E+00 [=] ATM     Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.86146891E+01   1.11018383E+02   9.93917155E+01   1.00176910E+05  Hydrogen
  3.66868155E+01   5.55131961E+01   4.96994430E+01   7.95161268E+05  Oxygen
  5.42690025E+00   5.61000156E+00   5.02248064E+00   1.15465675E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95058817E+00   5.60799916E+00   5.02068795E+00   1.77998450E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47613771E+00   1.50108527E-03   1.34388050E-03   1.61413487E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   5.18420811E-07   4.64127943E-07   1.10020694E-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
 -1.02828867E-15  -2.95636061E-15  -2.64674862E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     461.868060856175      grams
    H2O MASS          347.822478666651      grams
    TDS(g/kg)         327.884450213538      g/kgH2O

  Specified Solution Density
    DENSITY           1188.81855435140      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388510138208740       liters
    TDS               293.545961799972      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                              WATER    8.31862E-01   7.78067E-01   0.9353        1.93072E+01   4.96954E+01   8.95273E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)             9.99250E+00   1.00000E+00   1.000         3.47562E+00   8.94601E+00   3.14941E+06
Na+                               Na+     5.61000E+00   5.28971E+00   0.9429        1.95128E+00   5.02248E+00   1.15466E+05
Cl-                               Cl-     5.60800E+00   5.28867E+00   0.9431        1.95059E+00   5.02069E+00   1.77998E+05
HCO3-                             HCO3-   1.00903E-03   3.73572E-04   0.3702        3.50963E-04   9.03356E-04   5.51202E+01
CO3=                              CO3=    4.90717E-04   1.27445E-05   2.5971E-02    1.70682E-04   4.39325E-04   2.63636E+01
OH-                               OH-     1.07447E-05   5.84190E-06   0.5437        3.73726E-06   9.61946E-06   1.63601E-01   -4.59E-08
CO2(aq)                           CO2(aq) 4.82702E-07   1.40153E-06   2.904         1.67895E-07   4.32150E-07   1.90188E-02   -8.67E-08
NpO2(CO3)2=-                      NpO2(CO3)2=-  3.14571E-07   8.14859E-12   2.5904E-05   1.09415E-07   2.81627E-07   1.09571E-01   2.59E-08
NpO2CO3-                          NpO2CO3-  1.33630E-07   2.43107E-07   1.819         4.64794E-08   1.19635E-07   3.93666E-02   4.47E-12
NpO2+                             NpO2+   3.86807E-08   7.69314E-08   1.989         1.34540E-08   3.46298E-08   9.31704E-03   -2.13E-08
NpO2(CO3)3=-=-                    NpO2(CO3)3=-=-  3.13656E-08   2.48770E-17   7.9313E-10   1.09097E-08   2.80808E-08   1.26104E-02   4.49E-08
H+                                H+      3.42512E-10   1.34216E-09   3.919         1.19134E-10   3.06642E-10   3.09064E-07   -2.55E-08
NpO2OH(aq)                        NpO2OH(aq)  1.73507E-10   1.73507E-10   1.000         6.03495E-11   1.55336E-10   4.44344E-05   4.70E-09
NpO2(OH)2-                        NpO2(OH)2-  1.63614E-13   4.88873E-14   0.2988        5.69085E-14   1.46479E-13   4.43921E-08   2.99E-08
Na3H(CO3)2.2H2O_____Trona                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -5.33E+00
Na2CO3.H2O_____Thermonatrite              0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.04E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.75E+00
Na2CO3.10H2O_____Natron                   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.71E+00
NaHCO3_____Nahcolite                      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.30E+00
NaCl_____Halite                           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.32E+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
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
Np02OH(amor)_____________Np02OH(amor)     0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.63E+00
Np02OH(aged)_____________Np02OH(aged)     0.00000E+00   1.00000E+00   1.000      0.00000E+00   0.00000E+00   0.00000E+00   -3.03E+00
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

pmH = -log[m(H+)]                  =      9.4653
pH = -log[a(H+)]     =      8.8722
Osmotic Coefficient=     1.241539
Equilibrium RH (%) =    77.806749
Ionic Strength (m) =     5.610494
Density, kg/m3     =     1188.82

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

Total G/RT=     -4.63548129E+03
Flashing Titration #            6
# inversions for batch pblm            17
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
     Pressure=      1.00000E+00 [=] ATM     Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

 3.86270051E+01   1.11018410E+02   9.93919460E+01   1.00177142E+05  Hydrogen
 3.66936391E+01   5.55151239E+01   4.97012721E+01   7.95190533E+05  Oxygen
 5.42752260E+00   5.61000344E+00   5.02249276E+00   1.15465953E+05  Sodium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
 1.95076678E+00   5.60672579E+00   5.01955836E+00   1.77958403E+05  Chlorine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
 3.47635958E+00   2.13880634E-03   1.91481868E-03   2.29988871E+01  Carbon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
 3.47561578E+00   1.02583551E-06   9.18404325E-07   2.17706092E-01  Np(V)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
-9.45337050E-16  -2.71700630E-15  -2.43246632E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS     462.013014691340      grams
   H2O MASS          347.933330580303      grams
   TDS(g/kg)         327.877998698107      g/kgH2O

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

 Solution Parameters Based on Specified Density
   SOLUTION VOL      0.388633149984603     liters
   TDS               293.540795775029      g/l

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


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

 H2O                              WATER      8.31870E-01   7.78092E-01   0.9354        1.93133E+01   4.96955E+01   8.95274E+05
 NaNpO2CO3(s)_____NaNpO2CO3(s)               9.98931E+00   1.00000E+00   1.000         3.47562E+00   8.94318E+00   3.14841E+06
 Na+                              Na+        5.61000E+00   5.28932E+00   0.9428        1.95191E+00   5.02249E+00   1.15466E+05
 Cl-                              Cl-        5.60673E+00   5.28679E+00   0.9429        1.95077E+00   5.01956E+00   1.77958E+05
 CO3=                             CO3=       1.11398E-03   2.89293E-05   2.5969E-02    3.87591E-04   9.97318E-04   5.98482E+01
 HCO3-                            HCO3-      1.02256E-03   3.78536E-04   0.3702        3.55784E-04   9.15475E-04   5.58596E+01
 OH-                              OH-        2.40684E-05   1.30873E-05   0.5438        8.37419E-06   2.15478E-05   3.66470E-01   -4.86E-09
 Np02(CO3)2=-                     Np02(CO3)2=-  7.13649E-07   1.84983E-11   2.5921E-05    2.48302E-07   6.38912E-07   2.48578E-01   9.95E-09
 CO2(aq)                          CO2(aq)    2.18328E-07   6.33927E-07   2.904         7.59637E-08   1.95464E-07   8.60232E-03   -3.58E-08
 Np02CO3-                         Np02CO3-   1.33654E-07   2.43125E-07   1.819         4.65026E-08   1.19657E-07   3.93738E-02   1.56E-12
 Np02(CO3)3==-                    Np02(CO3)3==-  1.61312E-07   1.28193E-16   7.9469E-10    5.61257E-08   1.44418E-07   6.48546E-02   1.97E-08
 Np02+                            Np02+      1.70494E-08   3.38938E-08   1.988         5.93207E-09   1.52639E-08   4.10671E-03   -9.14E-09
 H+                               H+         1.52979E-10   5.99129E-10   3.916         5.32265E-11   1.36958E-10   1.38040E-07   -1.97E-08
 Np02OH(aq)                       Np02OH(aq) 1.71249E-10   1.71249E-10   1.000         5.95833E-11   1.53315E-10   4.38564E-05   1.06E-08
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
NpO2(OH)2-              NpO2(OH)2-     3.61806E-13   1.08095E-13   0.2988       1.25884E-13   3.23915E-13   9.81663E-08    3.03E-08
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
Na2CO3.H2O_____Thermonatrite           0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.68E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate     0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.39E+00
Na2CO3.10H2O_____________Natron        0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.36E+00
NaHCO3_____________Nahcolite           0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -2.30E+00
NaCl_____________Halite                0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED     0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -9.32E+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(amor)_____NpO2OH(amor)          0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.63E+00
NpO2OH(aged)_____NpO2OH(aged)          0.00000E+00   1.00000E+00    1.000       0.00000E+00   0.00000E+00   0.00000E+00   -3.04E+00
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

pmH = -log[m(H+)]                =      9.8154
pH = -log[a(H+)]     =      9.2225
Osmotic Coefficient=    1.241451
Equilibrium RH (%) =   77.809217
Ionic Strength (m) =    5.611121
Density, kg/m3     =    1188.82

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

Total G/RT=    -4.63619544E+03
Flashing Titration #           7
# inversions for batch pblm           17
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFP94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.86445565E+01   1.11018446E+02   9.93922712E+01   1.00177470E+05  Hydrogen
  3.67033634E+01   5.55178692E+01   4.97038762E+01   7.95232197E+05  Oxygen
  5.42840953E+00   5.61000623E+00   5.02251004E+00   1.15466351E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95102131E+00   5.60491242E+00   5.01794966E+00   1.77901369E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47667578E+00   3.04711826E-03   2.72801516E-03   3.27661900E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   1.94421849E-06   1.74061427E-06   4.12609480E-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
 -1.06779239E-15  -3.06756405E-15  -2.74631980E-15   0.00000000E+00  Electron
                                                    0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     462.219612785916      grams
    H2O MASS          348.091311120339      grams
    TDS(g/kg)         327.868860898172      g/kgH2O

  Specified Solution Density
    DENSITY           1188.81056561769      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388808466339423       liters
    TDS               293.533478681879      g/l

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


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                          WATER    8.31881E-01   7.78127E-01   0.9354        1.93221E+01   4.96957E+01   8.95277E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)         9.98478E+00   1.00000E+00    1.000        3.47562E+00   8.93914E+00   3.14699E+06
Na+                           Na+     5.61001E+00   5.28876E+00   0.9427        1.95279E+00   5.02251E+00   1.15466E+05
Cl-                           Cl-     5.60491E+00   5.28411E+00   0.9428        1.95102E+00   5.01795E+00   1.77901E+05
CO3=                          CO3=    2.00201E-03   5.19857E-05   2.5967E-02    6.96883E-04   1.79236E-03   1.07558E+02
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
HCO3-                          HCO3-      1.04073E-03  3.85192E-04  0.3701      3.62268E-04  9.31738E-04  5.68519E+01
OH-                            OH-        4.24988E-05  2.31125E-05  0.5438      1.47935E-05  3.80482E-05  6.47098E-01  -6.18E-08
NpO2(CO3)2=-          NpO2(CO3)2=-        1.28137E-06  3.32447E-11  2.5945E-05  4.46032E-07  1.14718E-06  4.46327E-01   4.81E-08
NpO2(CO3)3==-         NpO2(CO3)3==-       5.19502E-07  4.13999E-16  7.9692E-10  1.80834E-07  4.65098E-07  2.08864E-01   1.06E-07
CO2(aq)                        CO2(aq)    1.25799E-07  3.65269E-07  2.904       4.37894E-08  1.12625E-07  4.95659E-03  -3.39E-07
NpO2CO3-              NpO2CO3-            1.33688E-07  2.43151E-07  1.819       4.65356E-08  1.19688E-07  3.93840E-02   1.10E-12
NpO2+                          NpO2+      9.49498E-09  1.88634E-08  1.987       3.30512E-09  8.50064E-09  2.28707E-03  -4.03E-08
H+                             H+         8.66954E-11  3.39269E-10  3.913       3.01779E-11  7.76164E-11  7.82296E-08  -1.47E-07
NpO2OH(aq)            NpO2OH(aq)          1.68316E-10  1.68316E-10  1.000       5.85892E-11  1.50689E-10  4.31052E-05   1.04E-07
NpO2(OH)2-            NpO2(OH)2-          6.28105E-13  1.87627E-13  0.2987      2.18638E-13  5.62328E-13  1.70420E-07   2.44E-07
Na3H(CO3)2.2H2O_____________Trona         0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -4.70E+00
Na2CO3.H2O__________Thermonatrite         0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.43E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.14E+00
Na2CO3.10H2O_________________Natron       0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.10E+00
NaHCO3_____________________Nahcolite      0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -2.29E+00
NaCl_______________________Halite         0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -1.24E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -9.31E+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)_____________NpO2OH(amor)     0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.64E+00
NpO2OH(aged)_____________NpO2OH(aged)     0.00000E+00  1.00000E+00  1.000       0.00000E+00  0.00000E+00  0.00000E+00  -3.05E+00
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

pmH = -log[m(H+)]                  =      10.0620
pH = -log[a(H+)]     =       9.4695
Osmotic Coefficient=     1.241325
Equilibrium RH (%) =    77.812731
Ionic Strength (m) =     5.612017
Density, kg/m3     =     1188.81

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

Total G/RT=     -4.63721298E+03
Flashing Titration #            8
# inversions for batch pblm           23
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFP94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

 3.86695692E+01   1.11018496E+02   9.93927291E+01   1.00177932E+05  Hydrogen
 3.67172215E+01   5.55217779E+01   4.97075822E+01   7.95291491E+05  Oxygen
 5.42967348E+00   5.61001045E+00   5.02253469E+00   1.15466917E+05  Sodium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
 1.95138405E+00   5.60233091E+00   5.01565935E+00   1.77820171E+05  Chlorine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
 3.47712639E+00   4.34048558E-03   3.88595344E-03   4.66741868E+01  Carbon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
 3.47561578E+00   3.60501967E-06   3.22750493E-06   7.65074233E-01  Np(V)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  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
-4.02027671E-16  -1.15420235E-15  -1.03333521E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS     462.514079623513      grams
   H2O MASS          348.316456438668      grams
   TDS(g/kg)         327.855951316366      g/kgH2O

 Specified Solution Density
   DENSITY           1188.80395005085      kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL    0.389058330100373       liters
   TDS               293.523141261063      g/l

 Density based on TDS and NaCl solutions    1188.80395005085      g/l
 Percent relative error vs NaCl density    0.0000000000000000E+000 %
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

 Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
 H2O                              WATER        8.31897E-01   7.78177E-01   0.9354        1.93346E+01   4.96959E+01   8.95281E+05
 NaNpO2CO3(s)_____NaNpO2CO3(s)                 9.97832E+00   1.00000E+00   1.000         3.47561E+00   8.93340E+00   3.14497E+06
 Na+                              Na+          5.61001E+00   5.28798E+00   0.9426        1.95406E+00   5.02253E+00   1.15467E+05
 Cl-                              Cl-          5.60233E+00   5.28028E+00   0.9425        1.95138E+00   5.01566E+00   1.77820E+05
 CO3=                             CO3=         3.26656E-03   8.48095E-05   2.5963E-02    1.13780E-03   2.92449E-03   1.75496E+02
 HCO3-                            HCO3-        1.06541E-03   3.94227E-04   0.3700        3.71098E-04   9.53837E-04   5.82004E+01
 OH-                              OH-          6.77337E-05   3.68439E-05   0.5440        2.35928E-05   6.06407E-05   1.03133E+00   -3.65E-10
 NpO2(CO3)2=-          NpO2(CO3)2=-            2.08796E-06   5.42434E-11   2.5979E-05    7.27272E-07   1.86931E-06   7.27286E-01    2.37E-09
 NpO2(CO3)3==-         NpO2(CO3)3==-           1.37733E-06   1.10201E-15   8.0011E-10    4.79745E-07   1.23309E-06   5.53751E-01    4.86E-09
 CO2(aq)                          CO2(aq)      8.07635E-08   2.34511E-07   2.904         2.81313E-08   7.23060E-08   3.18217E-03   -1.78E-08
 NpO2CO3-                         NpO2CO3-     1.33737E-07   2.43187E-07   1.818         4.65827E-08   1.19732E-07   3.93986E-02    1.23E-12
 NpO2+                            NpO2+        5.82643E-09   1.15644E-08   1.985         2.02944E-09   5.21629E-09   1.40343E-03   -2.34E-09
 H+                               H+           5.44489E-11   2.12840E-10   3.909         1.89655E-11   4.87471E-11   4.91322E-08   -9.88E-09
 NpO2OH(aq)                       NpO2OH(aq)   1.64493E-10   1.64493E-10   1.000         5.72955E-11   1.47267E-10   4.21264E-05    7.54E-09
 NpO2(OH)2-                       NpO2(OH)2-   9.78743E-13   2.92306E-13   0.2987        3.40912E-13   8.76250E-13   2.65558E-07    1.74E-08
 Na3H(CO3)2.2H2O_____Trona                     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.48E+00
 Na2CO3.H2O_____Thermonatrite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.22E+00
 Na2CO3.7H2O____Na2CO3-Heptahydrate            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.93E+00
 Na2CO3.10H2O_____Natron                       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.89E+00
 NaHCO3_____Nahcolite                          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.28E+00
 NaCl_____Halite                               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.24E-01
 Na3NpO2(CO3)2(s)_DISABLED_DISABLED            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+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)_____NpO2OH(amor)                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.65E+00
 NpO2OH(aged)_____NpO2OH(aged)                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.06E+00
 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

 pmH = -log[m(H+)]                =     10.2640
 pH = -log[a(H+)]     =      9.6719
 Osmotic Coefficient=     1.241147
 Equilibrium RH (%) =    77.817733
 Ionic Strength (m) =     5.613297
 Density, kg/m3     =     1188.80

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

 Total G/RT=     -4.63866284E+03
 Flashing Titration #            9
 # inversions for batch pblm           23
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
 DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
      Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

 Elemental Abundances for Flash Problem

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

   3.87052148E+01    1.11018564E+02    9.93933709E+01    1.00178579E+05   Hydrogen
   3.67369708E+01    5.55273411E+01    4.97128537E+01    7.95375832E+05   Oxygen
   5.43147475E+00    5.61001696E+00    5.02256990E+00    1.15467727E+05   Sodium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Potassium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Magnesium
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Calcium
   1.95190099E+00    5.59865759E+00    5.01240002E+00    1.77704618E+05   Chlorine
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Sulfur
   3.47776855E+00    6.18147537E-03    5.53418864E-03    6.64711398E+01   Carbon
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   PosIon
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   NegIon
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Air
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Boron
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Bromine
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   TracerEl
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Th(IV)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Am(III)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   U(VI)
   3.47561578E+00    6.66349238E-06    5.96573175E-06    1.41416597E+00   Np(V)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   ClO4-(EL)
   0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00   Phosphorus
  -1.13087115E-15   -3.24368928E-15   -2.90402975E-15    0.00000000E+00   Electron
                                                                          Charge

   Solution Parameters, Calculated
     SOLUTION MASS     462.933810446950      grams
     H2O MASS          348.637323019311      grams
     TDS(g/kg)         327.837784084031      g/kgH2O

   Specified Solution Density
     DENSITY           1188.79464008680      kg/m^3 = g/l
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
   Solution Parameters Based on Specified Density
     SOLUTION VOL      0.389414449591688       liters
     TDS               293.508593601194        g/l

   Density based on TDS and NaCl solutions     1188.79464008680       g/l
   Percent relative error vs NaCl density     0.000000000000000E+000 %



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                  Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                WATER      8.31919E-01   7.78249E-01   0.9355        1.93524E+01   4.96961E+01   8.95286E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)                 9.96914E+00   1.00000E+00   1.000         3.47561E+00   8.92523E+00   3.14209E+06
Na+                                Na+        5.61002E+00   5.28690E+00   0.9424        1.95586E+00   5.02257E+00   1.15468E+05
Cl-                                Cl-        5.59866E+00   5.27483E+00   0.9422        1.95190E+00   5.01240E+00   1.77705E+05
CO3=                               CO3=       5.06627E-03   1.31507E-04   2.5957E-02    1.76629E-03   4.53576E-03   2.72187E+02
HCO3-                              HCO3-      1.09867E-03   4.06389E-04   0.3699        3.83037E-04   9.83623E-04   6.00178E+01
OH-                                OH-        1.01865E-04   5.54263E-05   0.5441        3.55141E-05   9.11987E-05   1.55104E+00   -1.77E-10
NpO2(CO3)2=-                       NpO2(CO3)2=-  3.23222E-06  8.41283E-11   2.6028E-05    1.12687E-06   2.89376E-06   1.12586E+00   8.12E-10
NpO2(CO3)3==-                      NpO2(CO3)3==- 3.29354E-06  2.65024E-15   8.0468E-10    1.14825E-06   2.94866E-06   1.32417E+00   1.75E-09
CO2(aq)                            CO2(aq)    5.53405E-08   1.60697E-07   2.904         1.92938E-08   4.95456E-08   2.18049E-03   -9.24E-09
NpO2CO3-                           NpO2CO3-   1.33806E-07   2.43236E-07   1.818         4.66498E-08   1.19795E-07   3.94192E-02   5.06E-13
NpO2+                              NpO2+      3.76324E-09   7.45944E-09   1.982         1.31200E-09   3.36917E-09   9.06466E-04   -7.98E-10
H+                                 H+         3.62550E-11   1.41496E-10   3.903         1.26398E-11   3.24586E-11   3.27150E-08   -4.95E-09
NpO2OH(aq)                         NpO2OH(aq) 1.59617E-10   1.59617E-10   1.000         5.56486E-11   1.42903E-10   4.08781E-05   4.15E-09
NpO2(OH)2-                         NpO2(OH)2- 1.42919E-12   4.26699E-13   0.2986        4.98268E-13   1.27953E-12   3.87777E-07   9.11E-09
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
Na2CO3.H2O_____Thermonatrite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.03E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.74E+00
Na2CO3.10H2O_____Natron                       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.70E+00
NaHCO3_____Nahcolite                          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.26E+00
NaCl_____Halite                               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.25E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+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)_____NpO2OH(amor)                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.66E+00
NpO2OH(aged)_____NpO2OH(aged)                 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.07E+00
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

pmH = -log[m(H+)]                =     10.4406
pH = -log[a(H+)]     =      9.8493
Osmotic Coefficient=     1.240893
Equilibrium RH (%) =    77.824850
Ionic Strength (m) =     5.615126
Density, kg/m3     =     1188.79

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

Total G/RT=     -4.64072873E+03
Flashing Titration #           10
# inversions for batch pblm           22
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=      1.00000E+00 [=] ATM     Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.87560135E+01   1.11018653E+02   9.93942650E+01   1.00179480E+05  Hydrogen
  3.67651156E+01   5.55352555E+01   4.97203463E+01   7.95495709E+05  Oxygen
  5.43404174E+00   5.61002728E+00   5.02262026E+00   1.15468885E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95263769E+00   5.59343408E+00   5.00776448E+00   1.77540274E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47868370E+00   8.80060113E-03   7.87911990E-03   9.46361091E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   1.23872216E-05   1.10901974E-05   2.62891134E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -6.72313767E-16  -1.92587840E-15  -1.72422617E-15   0.00000000E+00  Charge
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  Solution Parameters, Calculated
    SOLUTION MASS     463.532138924454      grams
    H2O MASS          349.094609954685      grams
    TDS(g/kg)         327.812362913952      g/kgH2O

  Specified Solution Density
    DENSITY           1188.78161259327      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.389922029424127       liters
    TDS               293.488236965687      g/l

  Density based on TDS and NaCl solutions    1188.78161259327      g/l
  Percent relative error vs NaCl density    0.0000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                WATER    8.31951E-01   7.78350E-01   0.9356        1.93778E+01   4.96966E+01   8.95293E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)               9.95607E+00   1.00000E+00   1.000         3.47561E+00   8.91361E+00   3.13800E+06
Na+                                Na+      5.61003E+00   5.28539E+00   0.9421        1.95843E+00   5.02262E+00   1.15469E+05
Cl-                                Cl-      5.59343E+00   5.26704E+00   0.9416        1.95264E+00   5.00776E+00   1.77540E+05
CO3=                               CO3=     7.62562E-03   1.97880E-04   2.5949E-02    2.66206E-03   6.82717E-03   4.09693E+02
HCO3-                              HCO3-    1.14291E-03   4.22533E-04   0.3697        3.98983E-04   1.02324E-03   6.24350E+01
OH-                                OH-      1.47379E-04   8.02242E-05   0.5443        5.14493E-05   1.31948E-04   2.24408E+00   -2.23E-08
NpO2(CO3)2=-                       NpO2(CO3)2=-  4.85191E-06   1.26624E-10   2.6098E-05    1.69378E-06   4.34388E-06   1.69005E+00   1.77E-08
NpO2(CO3)3==-                      NpO2(CO3)3==-  7.39875E-06   6.00222E-15   8.1125E-10    2.58286E-06   6.62405E-06   2.97469E+00   3.56E-08
CO2(aq)                            CO2(aq)  3.97510E-08   1.15435E-07   2.904         1.38769E-08   3.55888E-08   1.56626E-03   -3.82E-07
NpO2CO3-                           NpO2CO3- 1.33905E-07   2.43306E-07   1.817         4.67454E-08   1.19884E-07   3.94486E-02   2.95E-11
NpO2+                              NpO2+    2.50641E-09   4.95882E-09   1.978         8.74975E-10   2.24398E-09   6.03735E-04   -1.78E-08
H+                                 H+       2.51081E-11   9.77709E-11   3.894         8.76512E-12   2.24792E-11   2.26567E-08   -1.28E-07
NpO2OH(aq)                         NpO2OH(aq)  1.53583E-10   1.53583E-10   1.000         5.36149E-11   1.37502E-10   3.93329E-05   1.10E-07
NpO2(OH)2-                         NpO2(OH)2-  1.99131E-12   5.94256E-13   0.2984        6.95155E-13   1.78281E-12   5.40300E-07   2.38E-07
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
Na2CO3.H2O_____Thermonatrite                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.85E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.56E+00
Na2CO3.10H2O_____Natron                     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+00
NaHCO3_____Nahcolite                        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.25E+00
NaCl_____Halite                             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.26E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+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)_____NpO2OH(amor)               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.68E+00
NpO2OH(aged)_____NpO2OH(aged)               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.09E+00
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

pmH = -log[m(H+)]                  =     10.6002
pH = -log[a(H+)]     =     10.0098
Osmotic Coefficient=    1.240532
Equilibrium RH (%) =   77.834968
Ionic Strength (m) =    5.617741
Density, kg/m3     =    1188.78

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

Total G/RT=    -4.64367246E+03
Flashing Titration #          11
# inversions for batch pblm          22
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,F91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.88284068E+01   1.11018771E+02   9.93954996E+01   1.00180724E+05  Hydrogen
  3.68052248E+01   5.55465070E+01   4.97309848E+01   7.95665918E+05  Oxygen
  5.43769997E+00   5.61004415E+00   5.02269243E+00   1.15470544E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95368755E+00   5.58601315E+00   5.00117739E+00   1.77306742E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47998788E+00   1.25239828E-02   1.12127662E-02   1.34676535E+02  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  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   2.32128943E-05   2.07825866E-05   4.92647476E+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
 -8.43194194E-16  -2.41087366E-15  -2.15846374E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     464.385150217386      grams
    H2O MASS          349.746321818902      grams
    TDS(g/kg)         327.777080834729      g/kgH2O

  Specified Solution Density
    DENSITY           1188.76353136245      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.390645521977908       liters
    TDS               293.459983409119      g/l

  Density based on TDS and NaCl solutions    1188.76353136245      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                WATER    8.31997E-01   7.78493E-01   0.9357        1.94140E+01   4.96971E+01   8.95304E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.93751E+00   1.00000E+00   1.000         3.47561E+00   8.89709E+00   3.13218E+06
Na+                                Na+      5.61004E+00   5.28333E+00   0.9418        1.96209E+00   5.02269E+00   1.15471E+05
Cl-                                Cl-      5.58601E+00   5.25591E+00   0.9409        1.95369E+00   5.00118E+00   1.77307E+05
CO3=                               CO3=     1.12609E-02   2.92079E-04   2.5937E-02    3.93846E-03   1.00819E-02   6.05009E+02
HCO3-                              HCO3-    1.20082E-03   4.43607E-04   0.3694        4.19981E-04   1.07510E-03   6.55992E+01
OH-                                OH-      2.07123E-04   1.12810E-04   0.5447        7.24404E-05   1.85438E-04   3.15380E+00   -2.25E-09
NpO2(CO3)2=-              NpO2(CO3)2=-      7.13717E-06   1.86975E-10   2.6197E-05    2.49620E-06   6.38993E-06   2.48610E+00    4.21E-09
NpO2(CO3)3==-             NpO2(CO3)3==-     1.59398E-05   1.30821E-14   8.2072E-10    5.57490E-06   1.42710E-05   6.40874E+00    8.72E-09
CO2(aq)                          CO2(aq)    2.96765E-08   8.61856E-08   2.904         1.03792E-08   2.65695E-08   1.16932E-03   -9.22E-08
NpO2CO3-                      NpO2CO3-      1.34044E-07   2.43401E-07   1.816         4.68815E-08   1.20010E-07   3.94902E-02    8.14E-12
NpO2+                            NpO2+      1.70329E-09   3.36086E-09   1.973         5.95718E-10   1.52496E-09   4.10285E-04   -4.25E-09
NpO2OH(aq)                NpO2OH(aq)        1.46370E-10   1.46370E-10   1.000         5.11925E-11   1.31046E-10   3.74863E-05    4.11E-08
H+                                 H+       1.79163E-11   6.95424E-11   3.882         6.26615E-12   1.60405E-11   1.61672E-08   -4.53E-08
NpO2(OH)2-                NpO2(OH)2-        2.67040E-12   7.96388E-13   0.2982        9.33963E-13   2.39082E-12   7.24565E-07    8.64E-08
Na3H(CO3)2.2H2O_____________Trona           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.89E+00
Na2CO3.H2O___________Thermonatrite          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.68E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.39E+00
Na2CO3.10H2O_________________Natron         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.35E+00
NaHCO3_____________________Nahcolite        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.23E+00
NaCl_______________________Halite           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.27E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+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)_____________NpO2OH(amor)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.70E+00
NpO2OH(aged)_____________NpO2OH(aged)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.11E+00
HCl(aq).....to.titrate.acid.only            0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02

pmH = -log[m(H+)]                  =     10.7468
pH = -log[a(H+)]     =     10.1578
Osmotic Coefficient=     1.240021
Equilibrium RH (%) =    77.849336
Ionic Strength (m) =     5.621486
Density, kg/m3     =     1188.76

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

Total G/RT=     -4.64786705E+03
Flashing Titration #           12
# inversions for batch pblm           22
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFP94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.89315747E+01   1.11018923E+02   9.93971848E+01   1.00182423E+05  Hydrogen
  3.68623846E+01   5.55624877E+01   4.97460679E+01   7.95907238E+05  Oxygen
  5.44291331E+00   5.61007250E+00   5.02279611E+00   1.15472927E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95518372E+00   5.57548446E+00   4.99182884E+00   1.76975308E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.48184647E+00   1.78114648E-02   1.59469162E-02   1.91538411E+02  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   4.37690919E-05   3.91872342E-05   9.28926332E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.32033463E-15  -3.76512199E-15  -3.37097962E-15   0.00000000E+00  Charge

 Solution Parameters, Calculated
   SOLUTION MASS     465.601420606269      grams
   H2O MASS          350.675126352096      grams
   TDS(g/kg)         327.728674256700      g/kgH2O

 Specified Solution Density
   DENSITY           1188.73872346794      kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL    0.391676834795082       liters
   TDS               293.421218832869      g/l

 Density based on TDS and NaCl solutions    1188.73872346794      g/l
 Percent relative error vs NaCl density    0.000000000000000E+000 %



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                                WATER    8.32061E-01   7.78697E-01   0.9359        1.94655E+01   4.96979E+01   8.95318E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.91117E+00   1.00000E+00   1.000         3.47560E+00   8.87364E+00   3.12393E+06
Na+                                Na+      5.61007E+00   5.28057E+00   0.9413        1.96731E+00   5.02280E+00   1.15473E+05
Cl-                                Cl-      5.57548E+00   5.24002E+00   0.9398        1.95518E+00   4.99183E+00   1.76975E+05
CO3=                               CO3=     1.64154E-02   4.25480E-04   2.5920E-02    5.75648E-03   1.46970E-02   8.81956E+02
HCO3-                              HCO3-    1.27533E-03   4.70618E-04   0.3690        4.47227E-04   1.14183E-03   6.96709E+01
OH-                                OH-      2.84255E-04   1.54942E-04   0.5451        9.96812E-05   2.54499E-04   4.32833E+00   -1.42E-09
NpO2(CO3)2=-                NpO2(CO3)2=-    1.03463E-05   2.72515E-10   2.6339E-05    3.62818E-06   9.26320E-06   3.60399E+00    2.42E-09
NpO2(CO3)3==-               NpO2(CO3)3==-   3.32873E-05   2.77756E-14   8.3442E-10    1.16730E-05   2.98027E-05   1.33836E+01    5.14E-09
CO2(aq)                          CO2(aq)    2.29199E-08   6.65707E-08   2.904         8.03744E-09   2.05206E-08   9.03107E-04   -7.40E-08
NpO2CO3-                        NpO2CO3-    1.34242E-07   2.43528E-07   1.814         4.70755E-08   1.20190E-07   3.95491E-02    6.18E-12
NpO2+                              NpO2+    1.17432E-09   2.30833E-09   1.966         4.11805E-10   1.05139E-09   2.82874E-04   -2.46E-09
NpO2OH(aq)                    NpO2OH(aq)    1.38078E-10   1.38078E-10   1.000         4.84205E-11   1.23624E-10   3.53631E-05    3.39E-08
H+                                 H+       1.31074E-11   5.06455E-11   3.864         4.59643E-12   1.17353E-11   1.18280E-08   -3.64E-08
NpO2(OH)2-                    NpO2(OH)2-    3.46327E-12   1.03185E-12   0.2979        1.21448E-12   3.10073E-12   9.39711E-07    7.04E-08
Na3H(CO3)2.2H2O_____________Trona          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.70E+00
Na2CO3.H2O___________Thermonatrite         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.52E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.23E+00
Na2CO3.10H2O_____________Natron            0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.19E+00
NaHCO3_____________________Nahcolite       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.20E+00
NaCl_______________________Halite          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.28E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+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)_____________NpO2OH(amor)      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.73E+00
NpO2OH(aged)_____________NpO2OH(aged)      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.13E+00
HCl(aq).....to.titrate.acid.only           0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02

pmH = -log[m(H+)]                  =      10.8825
pH = -log[a(H+)]     =      10.2955
Osmotic Coefficient=     1.239297
Equilibrium RH (%) =    77.869707
Ionic Strength (m) =     5.626852
Density, kg/m3     =     1188.74

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

Total G/RT=     -4.65384406E+03
Flashing Titration #           13
# inversions for batch pblm           22
1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.6lmolal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (PRSR89,PRP90,P91,RPFR92,RPF94,RRPF94)
     Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
Elemental Abundances for Flash Problem

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

  3.90785996E+01   1.11019115E+02   9.93994493E+01   1.00184705E+05  Hydrogen
  3.69438430E+01   5.55851538E+01   4.97674088E+01   7.96248680E+05  Oxygen
  5.45034287E+00   5.61012129E+00   5.02294553E+00   1.15476363E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95731591E+00   5.56057489E+00   4.97858483E+00   1.76505768E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.48449515E+00   2.53082323E-02   2.26593804E-02   2.72161818E+02  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   8.26620364E-05   7.40103261E-05   1.75440146E+01  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Clo4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.25055944E-15  -3.55273740E-15  -3.18089495E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     467.335943430028      grams
    H2O MASS          351.998839687459      grams
    TDS(g/kg)         327.663306631854      g/kgH2O

  Specified Solution Density
    DENSITY           1188.70522197651      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.393147043346010       liters
    TDS               293.368869726079      g/l

  Density based on TDS and NaCl solutions    1188.70522197651      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                WATER    8.32153E-01   7.78985E-01   0.9361        1.95390E+01   4.96989E+01   8.95336E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.87386E+00   1.00000E+00   1.000         3.47559E+00   8.84042E+00   3.11224E+06
Na+                                 Na+     5.61012E+00   5.27693E+00   0.9406        1.97476E+00   5.02295E+00   1.15476E+05
Cl-                                 Cl-     5.56057E+00   5.21732E+00   0.9383        1.95732E+00   4.97858E+00   1.76506E+05
CO3=                                CO3=    2.37058E-02   6.13801E-04   2.5892E-02    8.34440E-03   2.12246E-02   1.27367E+03
HCO3-                               HCO3-   1.36956E-03   5.04583E-04   0.3684        4.82083E-04   1.22622E-03   7.48201E+01
OH-                                 OH-     3.82200E-04   2.08552E-04   0.5457        1.34534E-04   3.42198E-04   5.81986E+00   -1.17E-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   1.59E-09
NpO2(CO3)3==-                       NpO2(CO3)3==- 6.77047E-05  5.78442E-14  8.5436E-10  2.3832DE-05  6.06184E-05  2.72222E+01   3.46E-09
CO2(aq)                             CO2(aq) 1.82542E-08   5.30275E-08   2.905         6.42544E-09   1.63436E-08   7.19279E-04   -6.83E-08
NpO2CO3-                            NpO2CO3- 1.34522E-07  2.43696E-07   1.812         4.73516E-08   1.20442E-07   3.96323E-02   5.31E-13
NpO2+                               NpO2+   8.18986E-10   1.60121E-09   1.955         2.88282E-10   7.33267E-10   1.97283E-04   -1.64E-09
NpO2OH(aq)                          NpO2OH(aq) 1.28920E-10  1.28920E-10  1.000         4.53797E-11   1.15427E-10   3.30183E-05   3.16E-08
H+                                  H+      9.80463E-12   3.76405E-11   3.839         3.45122E-12   8.77844E-12   8.84779E-09   -3.32E-08
NpO2(OH)2-                          NpO2(OH)2- 4.35852E-12  1.29676E-12  0.2975        1.53420E-12   3.90234E-12   1.18365E-06   6.48E-08
Na3H(CO3)2.2H2O_____________Trona           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.51E+00
Na2CO3.H2O__________Thermonatrite           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.36E+00
Na2CO3.7H2O___Na2CO3-Heptahydrate           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.07E+00
Na2CO3.10H2O_____________Natron             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.03E+00
NaHCO3_____________Nahcolite                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.17E+00
NaCl_____________Halite                     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.31E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+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)_____________NpO2OH(amor)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.76E+00
NpO2OH(aged)_____________NpO2OH(aged)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.16E+00
HCl(aq).....to.titrate.acid.only            0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02

pmH = -log[m{H+}]                  =     11.0086
pH = -log[a(H+)]     =     10.4243
Osmotic Coefficient=     1.238276
Equilibrium RH (%) =    77.898521
Ionic Strength (m) =     5.634549
Density, kg/m3     =     1188.71

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

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
1523
1524 Total G/RT=     -4.66236092E+03
1525 Flashing Titration #          14
1526 # inversions for batch pblm          22
1527 1Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
1528 DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
1529 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
1530      Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin
1531
1532 Elemental Abundances for Flash Problem
1533
1534    Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
1535
1536   3.92881252E+01   1.11019354E+02   9.94024309E+01   1.00187710E+05  Hydrogen
1537   3.70599297E+01   5.56172351E+01   4.97975186E+01   7.96730419E+05  Oxygen
1538   5.46093075E+00   5.61020635E+00   5.02316152E+00   1.15481328E+05  Sodium
1539   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
1540   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
1541   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
1542   1.96035450E+00   5.53951836E+00   4.95987023E+00   1.75842279E+05  Chlorine
1543   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
1544   3.48826979E+00   3.59127333E-02   3.21548707E-02   3.86212152E+02  Carbon
1545   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
1546   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
1547   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
1548   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
1549   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
1550   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
1551   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
1552   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
1553   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
1554   3.47561578E+00   1.55346593E-04   1.39091324E-04   3.29713479E+01  Np(V)
1555   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
1556   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
1557  -8.00005678E-16  -2.26063508E-15  -2.02408511E-15   0.00000000E+00  Electron
1558                                                     0.00000000E+00  Charge
1559
1560   Solution Parameters, Calculated
1561     SOLUTION MASS     469.810029265032      grams
1562     H2O MASS          353.885368468197      grams
1563     TDS(g/kg)         327.576868460594      g/kgH2O
1564
1565   Specified Solution Density
1566     DENSITY           1188.66091947607      kg/m^3 = g/l
1567
1568   Solution Parameters Based on Specified Density
1569     SOLUTION VOL    0.395243102189405       liters
1570     TDS               293.299643066972      g/l
1571
1572   Density based on TDS and NaCl solutions    1188.66091947607      g/l
1573   Percent relative error vs NaCl density    0.000000000000000E+000 %
1574
1575
1576
1577 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
1578
1579 Species Name                          Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
1580
1581 H2O                          WATER    8.32282E-01   7.79391E-01   0.9365        1.96437E+01   4.97003E+01   8.95361E+05
1582 NaNpO2CO3(s)_____NaNpO2CO3(s)        9.82115E+00   1.00000E+00   1.000         3.47556E+00   8.79348E+00   3.09571E+06
1583 Na+                           Na+    5.61021E+00   5.27230E+00   0.9398        1.98537E+00   5.02316E+00   1.15481E+05
1584 Cl-                           Cl-    5.53952E+00   5.18493E+00   0.9360        1.96035E+00   4.95987E+00   1.75842E+05
1585 CO3=                          CO3=   3.39812E-02   8.78458E-04   2.5851E-02    1.20255E-02   3.04255E-02   1.82581E+03
1586 HCO3-                         HCO3-  1.48672E-03   5.46468E-04   0.3676        5.26128E-04   1.33115E-03   8.12230E+01
1587 OH-                           OH-    5.04619E-04   2.75741E-04   0.5464        1.78577E-04   4.51816E-04   7.68417E+00   -1.22E-09
1588 NpO2(CO3)2=-          NpO2(CO3)2=-   2.10028E-05   5.63525E-10   2.6831E-05    7.43260E-06   1.88051E-05   7.31643E+00    1.18E-09
1589 NpO2(CO3)3==-         NpO2(CO3)3==-  1.34208E-04   1.18584E-13   8.8359E-10    4.74943E-05   1.20165E-04   5.39629E+01    2.62E-09
1590 CO2(aq)                   CO2(aq)    1.49488E-08   4.34356E-08   2.906         5.29018E-09   1.33846E-08   5.89054E-04   -7.17E-08
1591 NpO2CO3-                NpO2CO3-     1.34916E-07   2.43910E-07   1.808         4.77447E-08   1.20798E-07   3.97494E-02    5.29E-12
1592 NpO2+                         NpO2+  5.77122E-10   1.11979E-09   1.940         2.04235E-10   5.16733E-10   1.39025E-04   -1.25E-09
1593 NpO2OH(aq)              NpO2OH(aq)    1.19205E-10   1.19205E-10   1.000         4.21850E-11   1.06732E-10   3.05311E-05    3.27E-08
1594 H+                            H+     7.48733E-12   2.84836E-11   3.804         2.64966E-12   6.70386E-12   6.75682E-09   -3.39E-08
1595 NpO2(OH)2-            NpO2(OH)2-     5.33952E-12   1.58534E-12   0.2969        1.88958E-12   4.78080E-12   1.44888E-06    6.67E-08
1596 Na3H(CO3)2.2H2O_____Trona             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.32E+00
1597 Na2CO3.H2O_____Thermonatrite          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.20E+00
1598 Na2CO3.7H2O____Na2CO3-Heptahydrate    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.91E+00
1599 Na2CO3.10H2O_____Natron               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.87E+00
1600 NaHCO3_____Nahcolite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.14E+00
1601 NaCl_____Halite                       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.34E-01
1602 Na3NpO2(CO3)2(s)_DISABLED_DISABLED    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+02
1603 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
1604 NpO2OH(amor)_____NpO2OH(amor)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.79E+00
1605 NpO2OH(aged)_____NpO2OH(aged)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.20E+00
1606 HCl(aq).....to.titrate.acid.only      0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02
1607
1608 pmH = -log[m(H+)]                =     11.1257
1609 pH = -log[a(H+)]     =     10.5454
1610 Osmotic Coefficient=     1.236838
1611 Equilibrium RH (%) =    77.939147
1612 Ionic Strength (m) =     5.645593
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
Density, kg/m3     =     1188.66

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

Total G/RT=     -4.67449693E+03
Flashing Titration #            15
# inversions for batch pblm           22
!Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
    Pressure=      1.00000E+00 [=] ATM      Temperature=      2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.95867206E+01   1.11019649E+02   9.94062599E+01   1.00191569E+05  Hydrogen
  3.72253652E+01   5.56624986E+01   4.98398335E+01   7.97407433E+05  Oxygen
  5.47601956E+00   5.61035435E+00   5.02347422E+00   1.15488517E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.96468480E+00   5.50989354E+00   4.93352227E+00   1.74908165E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.49364905E+00   5.08618173E-02   4.55413352E-02   5.46996977E+02  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   2.88102498E-04   2.57965074E-04   6.11501564E+01  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
 -1.86320143E-15  -5.22528680E-15  -4.67868728E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     473.339684533635      grams
    H2O MASS          356.574003417592      grams
    TDS(g/kg)         327.465491025424      g/kgH2O

  Specified Solution Density
    DENSITY           1188.60383111845      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.398231666549681       liters
    TDS              293.210437350984       g/l

  Density based on TDS and NaCl solutions    1188.60383111845      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                                WATER    8.32465E-01   7.79962E-01   0.9369        1.97930E+01   4.97021E+01   8.95393E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.74696E+00   1.00000E+00   1.000         3.47551E+00   8.72736E+00   3.07243E+06
Na+                                Na+      5.61035E+00   5.26665E+00   0.9387        2.00051E+00   5.02347E+00   1.15489E+05
Cl-                                Cl-      5.50989E+00   5.13884E+00   0.9327        1.96468E+00   4.93352E+00   1.74908E+05
CO3=                               CO3=     4.83971E-02   1.24807E-03   2.5788E-02    1.72571E-02   4.33344E-02   2.60046E+03
HCO3-                              HCO3-    1.63010E-03   5.97114E-04   0.3663        5.81251E-04   1.45958E-03   8.90593E+01
OH-                                OH-      6.55397E-04   3.58792E-04   0.5474        2.33698E-04   5.86939E-04   9.98054E+00   -2.54E-09
NpO2(CO3)2=-            NpO2(CO3)2=-        2.94209E-05   8.01487E-10   2.7242E-05    1.04907E-05   2.63433E-05   1.02493E+01    9.68E-10
NpO2(CO3)3==-           NpO2(CO3)3==-       2.58546E-04   2.39623E-13   9.2681E-10    9.21906E-05   2.31500E-04   1.03961E+02    2.18E-09
NpO2CO3-                      NpO2CO3-      1.35468E-07   2.44172E-07   1.802         4.83043E-08   1.21297E-07   3.99135E-02    6.09E-12
CO2(aq)                         CO2(aq)     1.25492E-08   3.64751E-08   2.907         4.47472E-09   1.12365E-08   4.94515E-04   -8.67E-08
NpO2+                             NpO2+     4.11022E-10   7.89015E-10   1.920         1.46560E-10   3.68027E-10   9.90165E-05   -1.07E-09
NpO2OH(aq)                  NpO2OH(aq)      1.09291E-10   1.09291E-10   1.000         3.89705E-11   9.78589E-11   2.79929E-05    3.69E-08
H+                                 H+       5.83272E-12   2.19064E-11   3.756         2.07980E-12   5.22258E-12   5.26384E-09   -3.80E-08
NpO2(OH)2-                  NpO2(OH)2-      6.38945E-12   1.89128E-12   0.2960        2.27831E-12   5.72107E-12   1.73384E-06    7.50E-08
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
Na2CO3.H2O_____Thermonatrite                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.05E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.76E+00
Na2CO3.10H2O_____________Natron             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.72E+00
NaHCO3_____________Nahcolite                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.10E+00
NaCl_____________Halite                     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.38E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+02
NaOH(aq).....to.titrate.base.only           0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.93E+02
```

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

```
1703 NpO2OH(amor)_________NpO2OH(amor)    0.00000E+00  1.00000E+00  1.000  0.00000E+00  0.00000E+00  0.00000E+00  -3.83E+00
1704 NpO2OH(aged)_________NpO2OH(aged)    0.00000E+00  1.00000E+00  1.000  0.00000E+00  0.00000E+00  0.00000E+00  -3.23E+00
1705 HCl(aq).......to.titrate.acid.only   0.00000E+00  0.00000E+00  1.000  0.00000E+00  0.00000E+00  0.00000E+00  -2.50E+02
1706
1707 pmH = -log[m(H+)]                =     11.2341
1708 pH = -log[a(H+)]     =     10.6594
1709 Osmotic Coefficient=    1.234823
1710 Equilibrium RH (%) =   77.996177
1711 Ionic Strength (m) =    5.661425
1712 Density, kg/m3     =    1188.60
1713
1714 NOTES:  - Water "molality" is mole fraction H2O in aqueous phase
1715         - Gas "molality" and "activity" are gas partial pressures
1716         - "Descriptor" means:
1717           *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
1718           *Saturation Index for minerals, SI=log10(IAP/Ksp)
1719           *log10(activity) for aqueous species with very small concentrations
1720           *log10(partial pressure) for gases
1721
1722 Total G/RT=    -4.69179003E+03
1723 TITRATE  file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LOG.TITRATE;1
1724 MOLES    file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LOG.MOLES;1
```

Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

See Table 27 for explanation of this listing.

```
 1  INPUT    file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LIN.IN;1
 2  INGUESS  file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LIN.INGUESS;1
 3  OUTPUT   file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LIN.OUT;2
 4  CHEMDAT  file name is U1:[SCBABB.FMT.USERGUIDE]FMT_HMW_NP_AM.CHEMDAT;1
 5  Temperature is Hard Coded as 298.15K
 6  Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.0
 7  DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 8  95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
 9
10
11  ********************************************************************************************************************************
12  *** ECHO PRINT OF "CHEMDAT" FILE WOULD BE HERE ***
13  ***               SEE APPENDIX J                ***
14  ********************************************************************************************************************************
15
16
17  TITRATION Problem:
18   -) Assigning all delta(y) to 0.1 m
19   -) Setting # of nodes in Y-direction to 3
20   -) Setting NONREACTIVE Porosity to 0.0
21
22
23
24  Specifying VARIABLE POROSITY for TITRATION Problem
25
26
27  Aqueous Density is a Function of Composition
28
29  RHOMIN   file name is U1:[SCBABB.FMT.USERGUIDE]FMT_HMW_NP_AM.RHOMIN;1
30
31  ********************************************************************************************************************************
32  *** TABLE OF MINERAL DENSITIES, KG/M^3 WOULD BE HERE ***
33  ***                SEE APPENDIX L                   ***
34  ********************************************************************************************************************************
35
36  GRID BLOCK VOLUMES, in liters
37   1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
38   1.00E+00  1.00E+00
39
40   1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
41   1.00E+00  1.00E+00
42
43   1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
44   1.00E+00  1.00E+00
45
46  # inversions for batch pblm           50
47 1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.0
48  DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
49  95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
50      Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin
51
52  Elemental Abundances for Flash Problem
53
54    Total Moles      Aq. Molality     Aq. Molarity     Aq. mg/liter
55
56    1.11017363E+02   1.11029658E+02   1.00100314E+02   1.00891107E+05  Hydrogen
57    6.15086815E+01   6.15154934E+01   5.54601388E+01   8.87328944E+05  Oxygen
58    5.61000000E+00   5.61062129E+00   5.05833276E+00   1.16289907E+05  Sodium
59    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
60    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
61    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
62    1.61000000E+00   1.61017830E+00   1.45167838E+00   5.14663538E+04  Chlorine
63    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
64    2.00000001E+00   2.00022150E+00   1.80332719E+00   2.16597629E+04  Carbon
65    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
66    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
67    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
68    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
69    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
70    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
71    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
72    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
73    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
74    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Np(V)
75    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
76    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
77    0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
78   -2.22044605E-15  -2.22069196E-15  -2.00209536E-15   0.00000000E+00  Charge
79
80    Solution Parameters, Calculated
81      SOLUTION MASS     1306.07033909890      grams
82      H2O MASS          999.889265717486      grams
```

Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
    TDS(g/kg)          306.214981877726       g/kgH2O

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

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

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



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                              Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                              WATER    8.57464E-01   8.59843E-01    1.003        5.55025E+01   5.00446E+01   9.01564E+05
Na+                                Na+    5.61062E+00   3.69881E+00    0.6593       5.61000E+00   5.05833E+00   1.16290E+05
CO3=                              CO3=    1.99407E+00   4.09214E-02    2.0522E-02   1.99385E+00   1.79778E+00   1.07884E+05
Cl-                                Cl-    1.61018E+00   1.06477E+00    0.6613       1.61000E+00   1.45168E+00   5.14664E+04
HCO3-                            HCO3-    6.14734E-03   1.59044E-03    0.2587       6.14666E-03   5.54222E-03   3.38170E+02
OH-                                OH-    6.14733E-03   4.86901E-03    0.7921       6.14665E-03   5.54221E-03   9.42580E+01    2.00E-11
CO2(aq)                        CO2(aq)    2.36876E-09   7.15913E-09    3.022        2.36850E-09   2.13559E-09   9.39868E-05   -2.12E-07
H+                                  H+    2.39954E-12   1.77959E-12    0.7416       2.39927E-12   2.16334E-12   2.18043E-09   -8.58E-08
Na3H(CO3)2.2H2O_____________Trona      0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.57E+00
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
NaCl_____________________________Halite 0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -9.75E-01
NaHCO3_____________________Nahcolite   0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -1.83E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate     0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -2.51E-01
Na2CO3.H2O_____________Thermonatrite   0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -7.99E-01
Na2CO3.10H2O_________________Natron    0.00000E+00   1.00000E+00    1.000        0.00000E+00   0.00000E+00   0.00000E+00   -8.30E-02

pmH = -log[m(H+)]                =     11.6199
pH = -log[a(H+)]    =     11.7497
Osmotic Coefficient=    0.908418
Equilibrium RH (%) =   85.984284
Ionic Strength (m) =    7.604695
Density, kg/m3     =     1177.64

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

Total G/RT=    -6.42133776E+03

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

shifting left by    4.644346544782S6
calling makenuv for allomorphic reactions
# inversions for batch pblm          75
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFP94,RRFP94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  1.11018363E+02   1.11017591E+02   9.93838868E+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   5.02297975E+00   1.78079701E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  1.00000000E+01   6.12839261E-04   5.48618892E-04   6.58946152E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  1.00000000E+01   6.12839261E-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
 -2.37316632E-15  -2.37314981E-15  -2.12446380E-15   0.00000000E+00  Charge
```

Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
  Solution Parameters, Calculated
    SOLUTION MASS     1328.11614865142      grams
    H2O MASS          1000.00695466819      grams
    TDS(g/kg)         328.106912108529      g/kgH2O

  Specified Solution Density
    DENSITY           1188.93254605477      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL      1.11706602116201      liters
    TDS               293.724084134187      g/l

  Density based on TDS and NaCl solutions    1188.93254605477      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                              WATER    8.31822E-01   7.77959E-01   0.9352        5.55091E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)    9.99932E+00   1.00000E+00   1.000         9.99939E+00   8.95147E+00   3.15133E+06
Cl-                                Cl-    5.61096E+00   5.29329E+00   0.9434        5.61100E+00   5.02298E+00   1.78080E+05
Na+                                Na+    5.61057E+00   5.29268E+00   0.9433        5.61061E+00   5.02263E+00   1.15469E+05
NpO2+                            NpO2+    6.12705E-04   1.21978E-03   1.991         6.12709E-04   5.48499E-04   1.47572E+02
CO2(aq)                        CO2(aq)    3.86103E-04   1.12115E-03   2.904         3.86106E-04   3.45643E-04   1.52117E+01
HCO3-                            HCO3-    2.26571E-04   8.38810E-05   0.3702        2.26573E-04   2.02829E-04   1.23760E+01    4.26E-09
NpO2CO3-                      NpO2CO3-    1.33526E-07   2.42971E-07   1.820         1.33527E-07   1.19534E-07   3.93334E-02   -1.99E-11
H+                                H+     1.21872E-06   4.78095E-06   3.923         1.21873E-06   1.09101E-06   1.09962E-03   -4.38E-08
CO3=                            CO3=     3.09384E-08   8.03342E-10   2.5966E-02    3.09386E-08   2.76963E-08   1.66203E-03   -1.62E-07
OH-                              OH-     3.01685E-09   1.63977E-09   0.5435        3.01687E-09   2.70071E-09   4.59318E-05    2.55E-08
NpO2OH(aq)                  NpO2OH(aq)    7.72186E-10   7.72186E-10   1.000         7.72191E-10   6.91267E-10   1.97740E-04    1.87E-07
NpO2(CO3)2=-              NpO2(CO3)2=-    1.98384E-11   5.13354E-16   2.5877E-05    1.98385E-11   1.77595E-11   6.90960E-06   -1.62E-07
NpO2(OH)2-                  NpO2(OH)2-    2.04382E-16   6.10703E-17   0.2988        2.04383E-16   1.82964E-16   5.54494E-11    2.13E-07
NpO2(CO3)3=4-            NpO2(CO3)3=4-    1.25197E-16   9.87896E-26   7.8908E-10    1.25198E-16   1.12077E-16   5.03310E-11   -3.23E-07
NpO2OH(aged)_____________NpO2OH(aged)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
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
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
Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NaCl_____________________________Halite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3___________________________Nahcolite 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
Na2CO3.10H2O_____________________Natron   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.H2O_____________Thermonatrite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na3H(CO3)2.2H2O_________________Trona     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
NpO2OH(amor)_____________NpO2OH(amor)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00

pmH = -log[m(H+)]                  =      5.9141
pH = -log[a(H+)]     =      5.3205
Osmotic Coefficient=     1.241871
Equilibrium RH (%) =    77.795863
Ionic Strength (m) =     5.611188
Density, kg/m3     =      1188.93

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

Total G/RT=     -1.33323084E+04
Flashing Titration #           1
# inversions for batch pblm          11
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  3.85857174E+01   1.11017591E+02   9.93838868E+01   1.00169020E+05  Hydrogen
  3.66707638E+01   5.55113597E+01   4.96942389E+01   7.95078006E+05  Oxygen
  5.42543623E+00   5.61057382E+00   5.02263316E+00   1.15469181E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95016801E+00   5.61096098E+00   5.02297975E+00   1.78079701E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47561578E+00   6.12839260E-04   5.48618892E-04   6.58946151E+00  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
```

Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   6.12839260E-04   5.48618892E-04   1.30049121E+02  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Cl04-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -6.94525850E-16  -1.99826754E-15  -1.78886601E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     461.602144251012      grams
    H2O MASS          347.563995068956      grams
    TDS(g/kg)         328.106912108175      g/kgH2O

  Specified Solution Density
    DENSITY           1188.93254605459      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388249228926247       liters
    TDS               293.724084133903      g/l

  Density based on TDS and NaCl solutions    1188.93254605459      g/l
  Percent relative error vs NaCl density    0.0000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                              WATER    8.31822E-01   7.77959E-01   0.9352        1.92928E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)    9.99932E+00   1.00000E+00   1.000         3.47540E+00   8.95147E+00   3.15133E+06
Cl-                               Cl-     5.61096E+00   5.29329E+00   0.9434        1.95017E+00   5.02298E+00   1.78080E+05
Na+                               Na+     5.61057E+00   5.29268E+00   0.9433        1.95003E+00   5.02263E+00   1.15469E+05
NpO2+                           NpO2+     6.12705E-04   1.21978E-03   1.991         2.12954E-04   5.48499E-04   1.47572E+02
CO2(aq)                       CO2(aq)     3.86103E-04   1.12115E-03   2.904         1.34196E-04   3.45643E-04   1.52117E+01
HCO3-                           HCO3-     2.26571E-04   8.38810E-05   0.3702        7.87481E-05   2.02829E-04   1.23760E+01   -6.17E-15
H+                                 H+     1.21872E-06   4.78095E-06   3.923         4.23582E-07   1.09101E-06   1.09962E-03    6.17E-15
NpO2CO3-                     NpO2CO3-     1.33526E-07   2.42971E-07   1.820         4.64090E-08   1.19534E-07   3.93334E-02    1.85E-14
CO3=                             CO3=     3.09384E-08   8.03343E-10   2.5966E-02    1.07531E-08   2.76963E-08   1.66203E-03    0.00E+00
OH-                               OH-     3.01685E-09   1.63977E-09   0.5435        1.04855E-09   2.70071E-09   4.59318E-05   -6.17E-15
NpO2OH(aq)                 NpO2OH(aq)     7.72186E-10   7.72186E-10   1.000         2.68384E-10   6.91267E-10   1.97740E-04    0.00E+00
NpO2(CO3)2=-             NpO2(CO3)2=-     1.98384E-11   5.13355E-16   2.5877E-05    6.89511E-12   1.77595E-11   6.90960E-06    0.00E+00
NpO2(OH)2-                 NpO2(OH)2-     2.04381E-16   6.10703E-17   0.2988        7.10356E-17   1.82964E-16   5.54494E-11    1.23E-14
NpO2(CO3)3==-           NpO2(CO3)3==-     1.25197E-16   9.87897E-26   7.8908E-10    4.35139E-17   1.12077E-16   5.03310E-11   -3.53E-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
NpO2OH(aged)_____________NpO2OH(aged)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
NpO2OH(amor)_____________NpO2OH(amor)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
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
Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NaCl_____________________________Halite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3___________________________Nahcolite 0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
Na2CO3.10H2O_____________________Natron   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.H2O_____________Thermonatrite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na3H(CO3)2.2H2O_____________Trona         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01

pmH = -log[m(H+)]                  =      5.9141
pH = -log[a(H+)]     =      5.3205
Osmotic Coefficient=     1.241871
Equilibrium RH (%) =    77.795863
Ionic Strength (m) =     5.611188
Density, kg/m3     =      1188.93

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

Total G/RT=     -4.63379813E+03

*****************************************************************************************
*** SUMMARY INFORMATION FOR ADDITION OF DV(2)...DV(14) WOULD BE HERE ***
*****************************************************************************************


 Flashing Titration #           15
 # inversions for batch pblm           23
1Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  PMT V2.0
 DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFP94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

 Elemental Abundances for Flash Problem

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

Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
  3.87258579E+01   1.11018601E+02   9.93937371E+01   1.00178948E+05  Hydrogen
  3.67484080E+01   5.55305592E+01   4.97159013E+01   7.95424591E+05  Oxygen
  5.43251790E+00   5.61002101E+00   5.02259034E+00   1.15468197E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.95220036E+00   5.59653330E+00   5.01051495E+00   1.77637786E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.47814044E+00   7.24644343E-03   6.48766141E-03   7.79233012E+01  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   8.79854005E-06   7.87723651E-06   1.86728474E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -9.13270924E-16  -2.61814885E-15  -2.34399998E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     463.176929136630      grams
    H2O MASS          348.823147935362      grams
    TDS(g/kg)         327.827387253719      g/kgH2O

  Specified Solution Density
    DENSITY           1188.78931208719      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.389620704381517       liters
    TDS               293.500268120485      g/l

  Density based on TDS and NaCl solutions    1188.78931208719      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                              WATER      8.31932E-01   7.78290E-01   0.9355        1.93627E+01   4.96963E+01   8.95289E+05
NaNpO2CO3(s)_____________NaNpO2CO3(s)      9.96382E+00   1.00000E+00   1.000         3.47561E+00   8.92050E+00   3.14043E+06
Na+                               Na+      5.61002E+00   5.28628E+00   0.9423        1.95691E+00   5.02259E+00   1.15468E+05
Cl-                               Cl-      5.59653E+00   5.27166E+00   0.9420        1.95220E+00   5.01051E+00   1.77638E+05
CO3=                              CO3=     6.10711E-03   1.58505E-04   2.5954E-02    2.13030E-03   5.46763E-03   3.28108E+02
HCO3-                             HCO3-    1.11706E-03   4.13103E-04   0.3698        3.89655E-04   1.00009E-03   6.10225E+01
OH-                               OH-      1.20768E-04   6.57227E-05   0.5442        4.21267E-05   1.08122E-04   1.83887E+00   -1.39E-10
NpO2(CO3)2=-           NpO2(CO3)2=-        3.89199E-06   1.01411E-10   2.6056E-05    1.35762E-06   3.48446E-06   1.35568E+00    5.14E-10
NpO2(CO3)3==-          NpO2(CO3)3==-       4.76942E-06   3.85055E-15   8.0734E-10    1.66368E-06   4.27001E-06   1.91755E+00    1.15E-09
CO2(aq)                          CO2(aq)   4.74407E-08   1.37761E-07   2.904         1.65484E-08   4.24731E-08   1.86923E-03   -7.11E-09
NpO2CO3-                      NpO2CO3-     1.33846E-07   2.43265E-07   1.817         4.66887E-08   1.19831E-07   3.94312E-02    3.15E-13
NpO2+                            NpO2+     3.12502E-09   6.18962E-09   1.981         1.09008E-09   2.79779E-09   7.5273BE-04   -5.05E-10
H+                                 H+      3.06048E-11   1.19335E-10   3.899         1.06757E-11   2.74002E-11   2.76166E-08   -3.76E-09
NpO2OH(aq)                    NpO2OH(aq)   1.57050E-10   1.57050E-10   1.000         5.47826E-11   1.40605E-10   4.02206E-05    3.26E-09
NpO2(OH)2-                    NpO2(OH)2-   1.66773E-12   4.97826E-13   0.2985        5.81743E-13   1.49310E-12   4.52501E-07    7.03E-09
Na3H(CO3)2.2H2O_____________Trona         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -4.19E+00
Na2CO3.H2O_____________Thermonatrite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.94E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.66E+00
Na2CO3.10H2O_________________Natron       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.62E+00
NaHCO3_____________________Nahcolite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.26E+00
NaCl_______________________Halite         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.25E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.31E+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
Np2OH(amor)_____________Np2OH(amor)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.67E+00
Np2OH(aged)_____________Np2OH(aged)       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.08E+00
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

pmH = -log[m(H+)]                  =      10.5142
pH = -log[a(H+)]     =       9.9232
Osmotic Coefficient=     1.240746
Equilibrium RH (%) =    77.828965
Ionic Strength (m) =     5.616187
Density, kg/m3     =      1188.79

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

Total G/RT=     -4.64192502E+03
TITRATE  file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM_LIN.TITRATE;2
```

Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

```
(43) MOLES    file name is U1:[SCRABB.FMT.USERGUIDE]NP_NACL_BM_LIN.MOLES;1
```

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

See Table 27 for explanation of this listing.

```
INPUT    file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM.IN;1
INGUESS  file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM.INGUESS;1
OUTPUT   file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM.OUT;1
CHEMDAT  file name is U1:[SCBABB.FMT.USERGUIDE]FMT_HMW_NP_AM.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)


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


TITRATION Problem:
 -) Assigning all delta(y) to 0.1 m
 -) Setting # of nodes in Y-direction to 3
 -) Setting NONREACTIVE Porosity to 0.0



Specifying VARIABLE POROSITY for TITRATION Problem


Aqueous Density is a Function of Composition

RHOMIN   file name is U1:[SCBABB.FMT.USERGUIDE]FMT_HMW_NP_AM.RHOMIN;1

**************************************************************************************************************
*** TABLE OF MINERAL DENSITIES, KG/M^3 WOULD BE HERE ***
***                  SEE APPENDIX L                  ***
**************************************************************************************************************

GRID BLOCK VOLUMES, in liters
 1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
 1.00E+00  1.00E+00

 1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
 1.00E+00  1.00E+00

 1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00  1.00E+00
 1.00E+00  1.00E+00

# inversions for batch pblm          50
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

  1.11017363E+02   1.11029658E+02   1.00100314E+02   1.00891107E+05  Hydrogen
  6.15086815E+01   6.15154934E+01   5.54601388E+01   8.87328944E+05  Oxygen
  5.61000000E+00   5.61062129E+00   5.05833276E+00   1.16289907E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.61000000E+00   1.61017830E+00   1.45167838E+00   5.14663538E+04  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  2.00000001E+00   2.00022150E+00   1.80332719E+00   2.16597629E+04  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -2.22044605E-15  -2.22069196E-15  -2.00209536E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS      1306.07033909890        grams
    H2O MASS           999.889265717486        grams
```

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

```
    TDS(g/kg)          306.214981877726       g/kgH2O

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

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

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



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                                 WATER   8.57464E-01   8.59843E-01    1.003        5.55025E+01   5.00446E+01   9.01564E+05
Na+                                   Na+   5.61062E+00   3.69881E+00   0.6593        5.61000E+00   5.05833E+00   1.16290E+05
CO3=                                  CO3=  1.99407E+00   4.09214E-02   2.0522E-02    1.99385E+00   1.79778E+00   1.07884E+05
Cl-                                   Cl-   1.61018E+00   1.06477E+00   0.6613        1.61000E+00   1.45168E+00   5.14664E+04
HCO3-                                 HCO3- 6.14734E-03   1.59044E-03   0.2587        6.14666E-03   5.54222E-03   3.38170E+02
OH-                                   OH-   6.14733E-03   4.86901E-03   0.7921        6.14665E-03   5.54221E-03   9.42580E+01    2.00E-11
CO2(aq)                             CO2(aq) 2.36876E-09   7.15913E-09    3.022        2.36850E-09   2.13559E-09   9.39868E-05   -2.12E-07
H+                                    H+    2.39954E-12   1.77959E-12   0.7416        2.39927E-12   2.16334E-12   2.18043E-09   -8.58E-08
Na3H(CO3)2.2H2O_____________Trona           0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.57E+00
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
NaCl_________________________Halite         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.75E-01
NaHCO3_____________________Nahcolite        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.83E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.51E-01
Na2CO3.H2O_____________Thermonatrite        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.99E-01
Na2CO3.10H2O_________________Natron         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.30E-02

pmH = -log[m(H+)]                 =     11.6199
pH = -log[a(H+)]     =     11.7497
Osmotic Coefficient=     0.908418
Equilibrium RH (%) =    85.984284
Ionic Strength (m) =     7.604695
Density, kg/m3     =      1177.64

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

Total G/RT=    -6.42133776E+03

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

shifting left by    4.64434654478256
calling makenuv for allomorphic reactions
# inversions for batch pblm          75
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.0
DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRP90,P91,RFFR92,RFF94,RRFF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

 1.11018363E+02   1.11017591E+02   9.93838868E+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   5.02297975E+00   1.78079701E+05  Chlorine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
 1.00000000E+01   6.12839261E-04   5.48618892E-04   6.58946152E+00  Carbon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
 0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
 1.00000000E+01   6.12839261E-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
-2.37316632E-15  -2.37314981E-15  -2.12446380E-15   0.00000000E+00  Charge
```

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

```
 Solution Parameters, Calculated
   SOLUTION MASS     1328.11614865142      grams
   H2O MASS          1000.006954668l9      grams
   TDS(g/kg)         328.106912108529      g/kgH2O

 Specified Solution Density
   DENSITY           1188.93254605477      kg/m^3 = g/l

 Solution Parameters Based on Specified Density
   SOLUTION VOL      1.11706602116201      liters
   TDS               293.724084134187      g/l

 Density based on TDS and NaCl solutions    1188.93254605477      g/l
 Percent relative error vs NaCl density     0.000000000000000E+000 %


 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

 H2O                              WATER    8.31822E-01   7.77959E-01   0.9352        5.55091E+01   4.96918E+01   8.95208E+05
 NaNpO2CO3(s)_____________NaNpO2CO3(s)    9.99932E+00   1.00000E+00   1.000         9.99939E+00   8.95147E+00   3.15133E+06
 Cl-                              Cl-      5.61096E+00   5.29329E+00   0.9434        5.61100E+00   5.02298E+00   1.78080E+05
 Na+                              Na+      5.61057E+00   5.29268E+00   0.9433        5.61061E+00   5.02263E+00   1.15469E+05
 NpO2+                            NpO2+    6.12705E-04   1.21978E-03   1.991         6.12709E-04   5.48499E-04   1.47572E+02
 CO2(aq)                          CO2(aq)  3.86103E-04   1.12115E-03   2.904         3.86106E-04   3.45643E-04   1.52117E+01
 HCO3-                            HCO3-    2.26571E-04   8.38810E-05   0.3702        2.26573E-04   2.02829E-04   1.23760E+01    4.26E-09
 NpO2CO3-                         NpO2CO3- 1.33526E-07   2.42971E-07   1.820         1.33527E-07   1.19534E-07   3.93334E-02   -1.99E-11
 H+                               H+       1.21872E-06   4.78095E-06   3.923         1.21873E-06   1.09101E-06   1.09962E-03   -4.38E-08
 CO3=                             CO3=     3.09384E-08   8.03342E-10   2.5966E-02    3.09386E-08   2.76963E-08   1.66203E-03   -1.62E-07
 OH-                              OH-      3.01685E-09   1.63977E-09   0.5435        3.01687E-09   2.70071E-09   4.59318E-05    2.55E-08
 NpO2OH(aq)                       NpO2OH(aq) 7.72186E-10  7.72186E-10   1.000         7.72191E-10   6.91267E-10   1.9774DE-04    1.87E-07
 NpO2(CO3)2=-                     NpO2(CO3)2=- 1.98384E-11 5.13354E-16   2.5877E-05    1.98385E-11   1.77595E-11   6.90960E-06   -1.62E-07
 NpO2(OH)2-                       NpO2(OH)2- 2.04382E-16  6.10703E-17   0.2988        2.04383E-16   1.82964E-16   5.54494E-11    2.13E-07
 NpO2(CO3)3==-                    NpO2(CO3)3==- 1.25197E-16 9.87896E-26  7.8908E-10    1.25198E-16   1.12077E-16   5.03310E-11   -3.23E-07
 NpO2OH(aged)_____________NpO2OH(aged)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
 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
 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
 Na3NpO2(CO3)2(s)_DISABLED_DISABLED        0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
 NaCl_____________________________Halite   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
 NaHCO3___________________________Nahcolite 0.00000E+00  1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
 Na2CO3.10H2O_____________________Natron   0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
 Na2CO3.7H2O___Na2CO3-Heptahydrate         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
 Na2CO3.H2O_____________Thermonatrite      0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
 Na3H(CO3)2.2H2O_________________Trona     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01
 NpO2OH(amor)_____________NpO2OH(amor)     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00

 pmH = -log[m(H+)]                  =       5.9141
 pH = -log[a(H+)]     =       5.3205
 Osmotic Coefficient=     1.241871
 Equilibrium RH (%) =    77.795863
 Ionic Strength (m) =     5.611188
 Density, kg/m3     =      1188.93

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

 Total G/RT=     -1.33323084E+04
 Flashing Titration #           1
 # inversions for batch pblm          11
 1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.0
 DATABASE:  HMW84/PW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
 95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RPFR92,RFF94,RRFF94)
     Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

 Elemental Abundances for Flash Problem

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

   3.85857174E+01   1.11017591E+02   9.93838868E+01   1.00169020E+05  Hydrogen
   3.66707638E+01   5.55113597E+01   4.96942389E+01   7.95078006E+05  Oxygen
   5.42543623E+00   5.61057382E+00   5.02263316E+00   1.15469181E+05  Sodium
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
   1.95016801E+00   5.61096098E+00   5.02297975E+00   1.78079701E+05  Chlorine
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
   3.47561578E+00   6.12839260E-04   5.48618892E-04   6.58946151E+00  Carbon
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
   0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
```

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

```
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   6.12839260E-04   5.48618892E-04   1.30049121E+02  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Cl04-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -6.94525850E-16  -1.99826754E-15  -1.78886601E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     461.602144251012      grams
    H2O MASS          347.563995068956      grams
    TDS(g/kg)         328.106912108175      g/kgH2O

  Specified Solution Density
    DENSITY           1188.93254605459      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.388249228926247       liters
    TDS               293.724084133903      g/l

  Density based on TDS and NaCl solutions    1188.93254605459      g/l
  Percent relative error vs NaCl density    0.0000000000000000E+000 %



TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

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

H2O                          WATER    8.31822E-01   7.77959E-01   0.9352        1.92928E+01   4.96918E+01   8.95208E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)         9.99932E+00   1.00000E+00   1.000         3.47540E+00   8.95147E+00   3.15133E+06
Cl-                           Cl-     5.61096E+00   5.29329E+00   0.9434        1.95017E+00   5.02298E+00   1.78080E+05
Na+                           Na+     5.61057E+00   5.29268E+00   0.9433        1.95003E+00   5.02263E+00   1.15469E+05
NpO2+                         NpO2+   6.12705E-04   1.21978E-03   1.991         2.12954E-04   5.48499E-04   1.47572E+02
CO2(aq)                       CO2(aq) 3.86103E-04   1.12115E-03   2.904         1.34196E-04   3.45643E-04   1.52117E+01
HCO3-                         HCO3-   2.26571E-04   8.38810E-05   0.3702        7.87481E-05   2.02829E-04   1.23760E+01   -6.17E-15
H+                            H+      1.21872E-06   4.78095E-06   3.923         4.23582E-07   1.09101E-06   1.09962E-03    6.17E-15
NpO2CO3-                      NpO2CO3- 1.33526E-07  2.42971E-07   1.820         4.64090E-08   1.19534E-07   3.93334E-02    1.85E-14
CO3=                          CO3=    3.09384E-08   8.03343E-10   2.5966E-02    1.07531E-08   2.76963E-08   1.66203E-03    0.00E+00
OH-                           OH-     3.01685E-09   1.63977E-09   0.5435        1.04855E-09   2.70071E-09   4.59318E-05   -6.17E-15
NpO2OH(aq)                    NpO2OH(aq) 7.72186E-10 7.72186E-10  1.000         2.68384E-10   6.91267E-10   1.97740E-04    0.00E+00
NpO2(CO3)2=-                  NpO2(CO3)2=- 1.98384E-11 5.13355E-16 2.5877E-05    6.89511E-12   1.77595E-11   6.90960E-06    0.00E+00
NpO2(OH)2-                    NpO2(OH)2- 2.04381E-16  6.10703E-17  0.2988        7.10356E-17   1.82964E-16   5.54494E-11    1.23E-14
NpO2(CO3)3==-                 NpO2(CO3)3==- 1.25197E-16 9.87897E-26 7.8908E-10    4.35139E-17   1.12077E-16   5.03310E-11   -3.53E-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
NpO2OH(aged)_____NpO2OH(aged)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.38E+00
NpO2OH(amor)_____NpO2OH(amor)         0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.98E+00
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
Na3NpO2(CO3)2(s)_DISABLED_DISABLED    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.36E+02
NaCl_____Halite                       0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.23E-01
NaHCO3_____Nahcolite                  0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.95E+00
Na2CO3.10H2O_____Natron               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.91E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate    0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -7.95E+00
Na2CO3.H2O_____Thermonatrite          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -8.24E+00
Na3H(CO3)2.2H2O_____Trona             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.02E+01

pmH = -log[m(H+)]                =      5.9141
pH = -log[a(H+)]     =      5.3205
Osmotic Coefficient=     1.241871
Equilibrium RH (%) =    77.795863
Ionic Strength (m) =     5.611188
Density, kg/m3     =      1188.93

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

Total G/RT=     -4.63379813E+03

*****************************************************************************************
*** SUMMARY INFORMATION FOR ADDITION OF DV(2)...DV(14) WOULD BE HERE ***
*****************************************************************************************


Flashing Titration #           15
# inversions for batch pblm           22
1Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRPF94)
    Pressure=     1.00000E+00 [=] ATM     Temperature=     2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

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

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

```
  3.95867206E+01   1.11019649E+02   9.94062599E+01   1.00191569E+05  Hydrogen
  3.72253652E+01   5.56624986E+01   4.98398335E+01   7.97407433E+05  Oxygen
  5.47601956E+00   5.61035435E+00   5.02347422E+00   1.15488517E+05  Sodium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Potassium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Magnesium
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Calcium
  1.96468480E+00   5.50989354E+00   4.93352227E+00   1.74908165E+05  Chlorine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Sulfur
  3.49364905E+00   5.08618173E-02   4.55413352E-02   5.46996977E+02  Carbon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  PosIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  NegIon
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Air
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Boron
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Bromine
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  TracerEl
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Th(IV)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Am(III)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  U(VI)
  3.47561578E+00   2.88102498E-04   2.57965074E-04   6.11501564E+01  Np(V)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  ClO4-(EL)
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Phosphorus
  0.00000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  Electron
 -1.85235941E-15  -5.19488071E-15  -4.65146187E-15   0.00000000E+00  Charge

  Solution Parameters, Calculated
    SOLUTION MASS     473.339684533635      grams
    H2O MASS          356.574003417592      grams
    TDS(g/kg)         327.465491025424      g/kgH2O

  Specified Solution Density
    DENSITY           1188.60383111845      kg/m^3 = g/l

  Solution Parameters Based on Specified Density
    SOLUTION VOL    0.398231666549681       liters
    TDS               293.210437350984      g/l

  Density based on TDS and NaCl solutions    1188.60383111845      g/l
  Percent relative error vs NaCl density    0.000000000000000E+000 %


TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name                                Molality      Activity      Act Coef      Total Moles   Molarity      mg/liter      Descriptor
H2O                              WATER      8.32465E-01   7.79962E-01   0.9369        1.97930E+01   4.97021E+01   8.95393E+05
NaNpO2CO3(s)_____NaNpO2CO3(s)               9.74696E+00   1.00000E+00   1.000         3.47551E+00   8.72736E+00   3.07243E+06
Na+                               Na+       5.61035E+00   5.26665E+00   0.9387        2.00051E+00   5.02347E+00   1.15489E+05
Cl-                               Cl-       5.50989E+00   5.13884E+00   0.9327        1.96468E+00   4.93352E+00   1.74908E+05
CO3=                              CO3=      4.83971E-02   1.24807E-03   2.5788E-02    1.72571E-02   4.33344E-02   2.60046E+03
HCO3-                             HCO3-     1.63010E-03   5.97114E-04   0.3663        5.81251E-04   1.45958E-03   8.90593E+01
OH-                               OH-       6.55397E-04   3.58792E-04   0.5474        2.33698E-04   5.86839E-04   9.98054E+00   -1.54E-09
NpO2(CO3)2=-                NpO2(CO3)2=-      2.94209E-05   8.01487E-10   2.7242E-05    1.04907E-05   2.63433E-05   1.02493E+01    9.68E-10
NpO2(CO3)3==-               NpO2(CO3)3==-     2.58546E-04   2.39623E-13   9.2681E-10    9.21906E-05   2.31500E-04   1.03961E+02    2.18E-09
NpO2CO3-                          NpO2CO3-  1.35468E-07   2.44172E-07   1.802         4.83043E-08   1.21297E-07   3.99135E-02    6.09E-12
CO2(aq)                           CO2(aq)   1.25492E-08   3.64751E-08   2.907         4.47472E-09   1.12365E-08   4.94515E-04   -8.67E-08
NpO2+                             NpO2+     4.11022E-10   7.89015E-10   1.920         1.46560E-10   3.68027E-10   9.90165E-05   -1.07E-09
NpO2OH(aq)                  NpO2OH(aq)      1.09291E-10   1.09291E-10   1.000         3.89705E-11   9.78589E-11   2.79929E-05    3.69E-08
H+                                H+        5.83272E-12   2.19064E-11   3.756         2.07980E-12   5.22258E-12   5.26384E-09   -3.80E-08
NpO2(OH)2-                  NpO2(OH)2-      6.38945E-12   1.89128E-12   0.2960        2.27831E-12   5.72107E-12   1.73384E-06    7.50E-08
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
Na2CO3.H2O_____Thermonatrite                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.05E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.76E+00
Na2CO3.10H2O_____________Natron             0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.72E+00
NaHCO3_____________Nahcolite                0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.10E+00
NaCl_____________Halite                     0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -1.38E-01
Na3NpO2(CO3)2(s)_DISABLED_DISABLED          0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -9.30E+02
NaOH(aq).....to.titrate.base.only           0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.93E+02
NpO2OH(amor)_____NpO2OH(amor)               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.83E+00
NpO2OH(aged)_____NpO2OH(aged)               0.00000E+00   1.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -3.23E+00
HCl(aq).....to.titrate.acid.only            0.00000E+00   0.00000E+00   1.000         0.00000E+00   0.00000E+00   0.00000E+00   -2.50E+02

pmH = -log[m(H+)]                =     11.2341
pH = -log[a(H+)]     =     10.6594
Osmotic Coefficient=     1.234823
Equilibrium RH (%) =    77.996177
Ionic Strength (m) =     5.661425
Density, kg/m3     =      1188.60

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

Total G/RT=    -4.69179003E+03
TITRATE  file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM.TITRATE;1
```

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

```
443 MOLES    file name is U1:[SCBABB.FMT.USERGUIDE]NP_NACL_BM.MOLES;1
```

Appendix Q: Sample Output File "BATCH_DOC.FOR088"

See Table 28 for explanation of this listing.

```
 1 5.506118174079332E+01 H2O                                  WATER 5.550868155779565E+01
 2 2.000000000000000E-01 Na+                                    Na+ 2.016254639034410E-01
 3 1.000000000000001E-02 K+                                     K+ 1.008127319517206E-02
 4 9.930829876074504E-05 Ca++                                   Ca++ 1.001154090354837E-04
 5 1.089876985084734E-08 Mg++                                   Mg++ 1.098734763576966E-08
 6 3.514119485249377E-08 MgOH+                                  MgOH+ 3.542679857127635E-08
 7 1.916539289681380E-13 H+                                     H+ 1.932115616855898E-13
 8 1.099999999999999E-01 Cl-                                    Cl- 1.108940051468925E-01
 9 9.999999999959653E-04 SO4=                                   SO4= 1.008127319513137E-03
10 4.035191240945192E-15 HSO4-                                  HSO4- 4.067986529473380E-15
11 9.800006626741904E-02 OH-                                    OH- 9.879654411868162E-02
12 1.092064419243065E-07 HCO3-                                  HCO3- 1.100939975711625E-07
13 9.919912603905744E-05 CO3=                                   CO3= 1.000053490322044E-04
14 2.193596324564590E-14 CO2(aq)                                CO2(aq) 2.211424382786093E-14
15 6.916147055733898E-07 CaCO3(aq)                              CaCO3(aq) 6.972356792683824E-07
16 5.279149790754905E-11 MgCO3(aq)                              MgCO3(aq) 5.322055127883555E-11
17 1.640770852300863E-11 B(OH)3(aq)                             B(OH)3(aq) 1.654105921272029E-11
18 9.989705247502765E-08 B(OH)4-                                B(OH)4- 1.007089477393192E-07
19 0.000000000000000E+00 B3O3(OH)4-                             B3O3(OH)4- 0.000000000000000E+00
20 0.000000000000000E+00 B4O5(OH)4=                             B4O5(OH)4= 0.000000000000000E+00
21 8.653368448896738E-11 CaB(OH)4+                              CaB(OH)4+ 8.723697139181022E-11
22 6.134836150886349E-15 MgB(OH)4+                              MgB(OH)4+ 6.184695924470303E-15
23 0.000000000000000E+00 Br-                                    Br- 0.000000000000000E+00
24 0.000000000000000E+00 ClO4-                 perchlorate ClO4- 0.000000000000000E+00
25 0.000000000000000E+00 NaOH(aq).....to.titrate.base.only      0.000000000000000E+00
26 0.000000000000000E+00 HCl(aq).....to.titrate.acid.only       0.000000000000000E+00
27 0.000000000000000E+00 HClO4(aq).....to.titrate.acid.only     0.000000000000000E+00
28 0.000000000000000E+00 PosIon.....POSITIVE.ION                0.000000000000000E+00
29 0.000000000000000E+00 NegIon.....NEGATIVE.ION                0.000000000000000E+00
30 0.000000000000000E+00 PosIon(OH)(aq).....to.titrate.base     0.000000000000000E+00
31 0.000000000000000E+00 HNegIon(aq).....to.titrate.acid        0.000000000000000E+00
32 0.000000000000000E+00 Tracer(aq).....conservative.tracer     0.000000000000000E+00
33 0.000000000000000E+00 H3PO4(aq)                              H3PO4(aq) 0.000000000000000E+00
34 0.000000000000000E+00 H2PO4-                                 H2PO4- 0.000000000000000E+00
35 0.000000000000000E+00 HPO4=                                  HPO4= 0.000000000000000E+00
36 0.000000000000000E+00 PO4=-                                  PO4=- 0.000000000000000E+00
37 0.000000000000000E+00 NpO2+                                  NpO2+ 0.000000000000000E+00
38 0.000000000000000E+00 NpO2OH(aq)                             NpO2OH(aq) 0.000000000000000E+00
39 0.000000000000000E+00 NpO2(OH)2-                             NpO2(OH)2- 0.000000000000000E+00
40 0.000000000000000E+00 NpO2CO3-                               NpO2CO3- 0.000000000000000E+00
41 0.000000000000000E+00 NpO2(CO3)2=-                           NpO2(CO3)2=- 0.000000000000000E+00
42 0.000000000000000E+00 NpO2(CO3)3==-                          NpO2(CO3)3==- 0.000000000000000E+00
43 0.000000000000000E+00 Am+++                                  Am+++ 0.000000000000000E+00
44 0.000000000000000E+00 AmCO3+                                 AmCO3+ 0.000000000000000E+00
45 0.000000000000000E+00 Am(CO3)2-                              Am(CO3)2- 0.000000000000000E+00
46 0.000000000000000E+00 Am(CO3)3=-                             Am(CO3)3=- 0.000000000000000E+00
47 0.000000000000000E+00 Am(OH)2+                               Am(OH)2+ 0.000000000000000E+00
48 0.000000000000000E+00 Am(OH)3(aq)                            Am(OH)3(aq) 0.000000000000000E+00
49 0.000000000000000E+00 Th++++                                 Th++++ 0.000000000000000E+00
50 0.000000000000000E+00 UO2++                                  U(VI)O2++ 0.000000000000000E+00
51 0.000000000000000E+00 NpO2OH(aged)_____NpO2OH(aged)          0.000000000000000E+00
52 0.000000000000000E+00 NpO2OH(amor)_____NpO2OH(amor)          0.000000000000000E+00
53 0.000000000000000E+00 NaNpO2CO3(s)_____NaNpO2CO3(s)          0.000000000000000E+00
54 0.000000000000000E+00 Na3NpO2(CO3)2(s)_DISABLED_DISABLED     0.000000000000000E+00
55 0.000000000000000E+00 AmOHCO3(c)_____AmOHCO3(c)              0.000000000000000E+00
56 0.000000000000000E+00 Am(OH)3(s)_____Am(OH)3(s)              0.000000000000000E+00
57 0.000000000000000E+00 NaAm(CO3)2.6H2O(c)_____                0.000000000000000E+00
58 0.000000000000000E+00 AmPO4(c)_____AmPO4(c)                  0.000000000000000E+00
59 0.000000000000000E+00 CaSO4_____Anhydrite                    0.000000000000000E+00
60 0.000000000000000E+00 NaK3(SO4)2__Aphthitalite/Glaserite     0.000000000000000E+00
61 0.000000000000000E+00 CaCl2.6H2O_____Antarcticite            0.000000000000000E+00
62 0.000000000000000E+00 CaCO3_____Aragonite                    0.000000000000000E+00
63 0.000000000000000E+00 K2SO4_____Arcanite                     0.000000000000000E+00
64 0.000000000000000E+00 MgCl2.6H2O_____Bischofite              0.000000000000000E+00
65 0.000000000000000E+00 Na2Mg(SO4)2.4H2O_____Bloedite          0.000000000000000E+00
66 9.999539072376642E-04 Mg(OH)2_____Brucite                    1.008080852144262E-03
67 0.000000000000000E+00 Na6CO3(SO4)2_____Burkeite              0.000000000000000E+00
68 0.000000000000000E+00 CaCO3_____Calcite                      0.000000000000000E+00
69 0.000000000000000E+00 CaCl2.4H2O_____CaCl2_Tetrahydrite      0.000000000000000E+00
70 0.000000000000000E+00 Ca4Cl2(OH)6.13H2O__CaOxychloride A     0.000000000000000E+00
71 0.000000000000000E+00 Ca2Cl2(OH)2.H2O____CaOxychloride B     0.000000000000000E+00
72 0.000000000000000E+00 KMgCl3.6H2O_____Carnallite             0.000000000000000E+00
73 0.000000000000000E+00 MgSO4.7H2O_____Epsomite                0.000000000000000E+00
74 0.000000000000000E+00 CaNa2(CO3)2.5H2O_____Gaylussite        0.000000000000000E+00
75 0.000000000000000E+00 Na2Ca(SO4)2_____Glauberite             0.000000000000000E+00
76 0.000000000000000E+00 CaSO4.2H2O_____Gypsum                  0.000000000000000E+00
77 0.000000000000000E+00 NaCl_____Halite                        0.000000000000000E+00
78 0.000000000000000E+00 MgSO4.6H2O_____Hexahydrite             0.000000000000000E+00
79 0.000000000000000E+00 KMgClSO4.3H2O_____Kainite              0.000000000000000E+00
80 0.000000000000000E+00 KHCO3_____Kalicinite                   0.000000000000000E+00
81 0.000000000000000E+00 MgSO4.H2O_____ Kieserite               0.000000000000000E+00
82 0.000000000000000E+00 K2Mg(SO4)2.4H2O_____Leonite            0.000000000000000E+00
```

Appendix Q: Sample Output File "BATCH_DOC.FOR088"

```
 83  0.000000000000000E+00 Na4Ca(SO4)3.2H2O_______Labile_Salt 0.000000000000000E+00
 84  0.000000000000000E+00 MgCO3_____________________Magnesite 0.000000000000000E+00
 85  0.000000000000000E+00 Mg2Cl(OH)3.4H2O______MgOxychloride 0.000000000000000E+00
 86  0.000000000000000E+00 KHSO4_____________________Mercallite 0.000000000000000E+00
 87  0.000000000000000E+00 Na2SO4.10H2O_____________Mirabilite 0.000000000000000E+00
 88  0.000000000000000E+00 K8H6(SO4)7_________________Misenite 0.000000000000000E+00
 89  0.000000000000000E+00 NaHCO3_____________________Nahcolite 0.000000000000000E+00
 90  0.000000000000000E+00 Na2CO3.10H2O_____________________Natron 0.000000000000000E+00
 91  0.000000000000000E+00 MgCO3.3H2O_____________Nesquehonite 0.000000000000000E+00
 92  0.000000000000000E+00 K2Mg(SO4)2.6H2O Picromerite/Schoen 0.000000000000000E+00
 93  0.000000000000000E+00 Na2Ca(CO3)2.2H2O_________Pirssonite 0.000000000000000E+00
 94  0.000000000000000E+00 K2MgCa2(SO4)4.2H2O______Polyhalite 0.000000000000000E+00
 95  0.000000000000000E+00 Ca(OH)2_____________________Portlandite 0.000000000000000E+00
 96  0.000000000000000E+00 K2CO3.3/2H2O___Potassium_Carbonate 0.000000000000000E+00
 97  0.000000000000000E+00 K8H4(CO3)6.3H2O___K-Sequicarbonate 0.000000000000000E+00
 98  0.000000000000000E+00 KNaCO3.6H2O_________K-Na-Carbonate 0.000000000000000E+00
 99  0.000000000000000E+00 K2NaH(CO3)2.2H2O___Potassium_Trona 0.000000000000000E+00
100  0.000000000000000E+00 K3H(SO4)2__Sesquipotassium_Sulfate 0.000000000000000E+00
101  0.000000000000000E+00 Na3H(SO4)2____Sesquisodium_Sulfate 0.000000000000000E+00
102  0.000000000000000E+00 Na2CO3.7H2O____Na2CO3-Heptahydrate 0.000000000000000E+00
103  0.000000000000000E+00 KCl_____________________________Sylvite 0.000000000000000E+00
104  0.000000000000000E+00 K2Ca(SO4)2.H2O_____________Syngenite 0.000000000000000E+00
105  0.000000000000000E+00 Mg2CaCl6.12H2O_________Tachyhydrite 0.000000000000000E+00
106  0.000000000000000E+00 Na2SO4_____________________Thenardite 0.000000000000000E+00
107  0.000000000000000E+00 Na2CO3.H2O_____________Thermonatrite 0.000000000000000E+00
108  0.000000000000000E+00 Na3H(CO3)2.2H2O_________________Trona 0.000000000000000E+00
109  0.000000000000000E+00 Na2B4O7.10H2O_____________ Borax 0.000000000000000E+00
110  0.000000000000000E+00 B(OH)3_____________Borix_Acid_Solid 0.000000000000000E+00
111  0.000000000000000E+00 KB5O8.4H2O____K-Pentaborate_(30_C) 0.000000000000000E+00
112  0.000000000000000E+00 K2B4O7.4H2O___K-Tetraborate_(30_C) 0.000000000000000E+00
113  0.000000000000000E+00 NaBO2.4H2O_______Sodium_Metaborate 0.000000000000000E+00
114  0.000000000000000E+00 NaB5O8.5H2O_____Sodium_Pentaborate 0.000000000000000E+00
115  0.000000000000000E+00 NaBO2.NaCl.2H2O___Teepleite_(20_C) 0.000000000000000E+00
```

Appendix R: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

See Table 29 for explanation of this listing.

```
Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NP94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

Titrant Volumes per Grid Block, in milliliters
   1              0.000000 mL
   2              0.100000 mL
   3              0.142510 mL
   4              0.203092 mL
   5              0.289427 mL
   6              0.412463 mL
   7              0.587802 mL
   8              0.837678 mL
   9              1.193777 mL
  10              1.701254 mL
  11              2.424462 mL
  12              3.455107 mL
  13              4.923883 mL
  14              7.017038 mL
  15             10.000000 mL


Titration Results, molal


      H2O           Na+           K+            Ca++          Mg++          MgOH+         H+            Cl-           SO4=
 1)  1.92928E+01  5.61057E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.21872E-06  5.61096E+00  0.00000E+00
 2)  1.92978E+01  5.61014E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.77346E-07  5.60993E+00  0.00000E+00
 3)  1.92999E+01  5.61003E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  2.58813E-07  5.60950E+00  0.00000E+00
 4)  1.93029E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  2.91065E-09  5.60889E+00  0.00000E+00
 5)  1.93072E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.42512E-10  5.60800E+00  0.00000E+00
 6)  1.93133E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.52979E-10  5.60673E+00  0.00000E+00
 7)  1.93221E+01  5.61001E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  8.66954E-11  5.60491E+00  0.00000E+00
 8)  1.93346E+01  5.61001E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.44489E-11  5.60233E+00  0.00000E+00
 9)  1.93524E+01  5.61002E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.62550E-11  5.59866E+00  0.00000E+00
10)  1.93778E+01  5.61003E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  2.51081E-11  5.59343E+00  0.00000E+00
11)  1.94140E+01  5.61004E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.79163E-11  5.58601E+00  0.00000E+00
12)  1.94655E+01  5.61007E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.31074E-11  5.57548E+00  0.00000E+00
13)  1.95390E+01  5.61012E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.80463E-12  5.56057E+00  0.00000E+00
14)  1.96437E+01  5.61021E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  7.48733E-12  5.53952E+00  0.00000E+00
15)  1.97930E+01  5.61035E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.83272E-12  5.50989E+00  0.00000E+00

      HSO4-         OH-           HCO3-         CO3=          CO2(aq)       CaCO3(aq)     MgCO3(aq)     B(OH)3(aq)    B(OH)4-
 1)  0.00000E+00  3.01685E-09  2.26571E-04  3.09384E-08  3.86103E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 2)  0.00000E+00  6.37029E-09  3.82212E-04  1.10196E-07  3.08476E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 3)  0.00000E+00  1.42123E-08  5.79856E-04  3.72979E-07  2.09763E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 4)  0.00000E+00  1.26397E-06  9.92660E-04  5.67888E-05  4.03745E-06  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 5)  0.00000E+00  1.07447E-05  1.00903E-03  4.90717E-04  4.82702E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 6)  0.00000E+00  2.40684E-05  1.02256E-03  1.11398E-03  2.18328E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 7)  0.00000E+00  4.24988E-05  1.04073E-03  2.00201E-03  1.25799E-07  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 8)  0.00000E+00  6.77337E-05  1.06541E-03  3.26656E-03  8.07635E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 9)  0.00000E+00  1.01865E-04  1.09867E-03  5.06627E-03  5.53405E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
10)  0.00000E+00  1.47379E-04  1.14291E-03  7.62562E-03  3.97510E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
11)  0.00000E+00  2.07123E-04  1.20082E-03  1.12609E-02  2.96765E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
12)  0.00000E+00  2.84255E-04  1.27533E-03  1.64154E-02  2.29199E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
13)  0.00000E+00  3.82200E-04  1.36956E-03  2.37058E-02  1.82542E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
14)  0.00000E+00  5.04619E-04  1.48672E-03  3.39812E-02  1.49488E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
15)  0.00000E+00  6.55397E-04  1.63010E-03  4.83971E-02  1.25492E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

      B3O3(OH)4-    B4O5(OH)4=    CaB(OH)4+     MgB(OH)4+     Br-           ClO4-         NaOH(aq)..... HCl(aq)...... HClO4(aq)....
 1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 4)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 5)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 6)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 7)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 8)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 9)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
10)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
11)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
12)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
13)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
14)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
15)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

      PosIon....... NegIon....... PosIon(OH)(aq HNegIon(aq).. Tracer(aq)... H3PO4(aq)    H2PO4-        HPO4=         PO4=-
 1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 4)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 5)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
```

Appendix R: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

83	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
84	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
85	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
86	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
87	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
88	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
89	12)	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*
90	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
91	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
92	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
93										
94		NpO2+	NpO2OH(aq)	NpO2(OH)2-	NpO2CO3-	NpO2(CO3)2=-	NpO2(CO3)3==-	Am+++	AmCO3+	Am(CO3)2-
95	1)	6.12705E-04	7.72186E-10	2.04381E-16	1.33526E-07	1.98384E-11	1.25197E-16	0.00000E+00	0.00000E+00	0.00000E+00
96	2)	1.72085E-04	4.57851E-10	2.55903E-16	1.33573E-07	7.06677E-11	1.58546E-15	0.00000E+00	0.00000E+00	0.00000E+00
97	3)	5.08519E-05	3.01826E-10	3.76383E-16	1.33591E-07	2.39201E-10	1.81540E-14	0.00000E+00	0.00000E+00	0.00000E+00
98	4)	3.34101E-07	1.76339E-10	1.95583E-14	1.33613E-07	3.64205E-08	4.20660E-10	0.00000E+00	0.00000E+00	0.00000E+00
99	5)	3.86807E-08	1.73507E-10	1.63614E-13	1.33630E-07	3.14571E-07	3.13656E-08	0.00000E+00	0.00000E+00	0.00000E+00
100	6)	1.70494E-08	1.71249E-10	3.61806E-13	1.33654E-07	7.13649E-07	1.61312E-07	0.00000E+00	0.00000E+00	0.00000E+00
101	7)	9.49498E-09	1.68316E-10	6.28105E-13	1.33688E-07	1.28137E-06	5.19502E-07	0.00000E+00	0.00000E+00	0.00000E+00
102	8)	5.82643E-09	1.64493E-10	9.78743E-13	1.33737E-07	2.08796E-06	1.37733E-06	0.00000E+00	0.00000E+00	0.00000E+00
103	9)	3.76324E-09	1.59617E-10	1.42919E-12	1.33806E-07	3.23222E-06	3.29354E-06	0.00000E+00	0.00000E+00	0.00000E+00
104	10)	2.50641E-09	1.53583E-10	1.99131E-12	1.33905E-07	4.85191E-06	7.39875E-06	0.00000E+00	0.00000E+00	0.00000E+00
105	11)	1.70329E-09	1.46370E-10	2.67040E-12	1.34044E-07	7.13717E-06	1.59398E-05	0.00000E+00	0.00000E+00	0.00000E+00
106	12)	1.17432E-09	1.38078E-10	3.46327E-12	1.34242E-07	1.03463E-05	3.32873E-05	0.00000E+00	0.00000E+00	0.00000E+00
107	13)	8.18986E-10	1.28920E-10	4.35852E-12	1.34522E-07	1.48219E-05	6.77047E-05	0.00000E+00	0.00000E+00	0.00000E+00
108	14)	5.77122E-10	1.19205E-10	5.33952E-12	1.34916E-07	2.10023E-05	1.34208E-04	0.00000E+00	0.00000E+00	0.00000E+00
109	15)	4.11022E-10	1.09291E-10	6.38945E-12	1.35468E-07	2.94209E-05	2.58546E-04	0.00000E+00	0.00000E+00	0.00000E+00
110										
111		Am(CO3)3=-	Am(OH)2+	Am(OH)3(aq)	Th++++	UO2++	NpO2OH(aged)_	NpO2OH(amor)_	NaNpO2CO3(s)_	Na3NpO2(CO3)2
112	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99932E+00	0.00000E+00
113	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99718E+00	0.00000E+00
114	3)	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*9.99622E+00*	*0.00000E+00*
115	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99473E+00	0.00000E+00
116	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99250E+00	0.00000E+00
117	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98931E+00	0.00000E+00
118	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98478E+00	0.00000E+00
119	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97832E+00	0.00000E+00
120	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96914E+00	0.00000E+00
121	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.95607E+00	0.00000E+00
122	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.93751E+00	0.00000E+00
123	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.91117E+00	0.00000E+00
124	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.87386E+00	0.00000E+00
125	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.82115E+00	0.00000E+00
126	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.74696E+00	0.00000E+00
127										
128		AmOHCO3(c)___	Am(OH)3(s)___	NaAm(CO3)2.6H	AmPO4(c)_____	CaSO4_____	NaK3(SO4)2__A	CaCl2.6H2O___	CaCO3_____	K2SO4_____
129	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
130	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
131	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
132	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
133	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
134	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
135	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
136	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
137	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
138	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
139	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*
140	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
141	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
142	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
143	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
144										
145		MgCl2.6H2O___	Na2Mg(SO4)2.4	Mg(OH)2_____	Na6CO3(SO4)2_	CaCO3_____	CaCl2.4H2O___	Ca4Cl2(OH)6.1	Ca2Cl2(OH)2.H	KMgCl3.6H2O__
146	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
147	2)	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
148	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
149	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
150	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
151	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
152	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
153	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
154	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
155	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
156	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
157	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
158	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
159	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
160	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
161										
162		MgSO4.7H2O___	CaNa2(CO3)2.5	Na2Ca(SO4)2__	CaSO4.2H2O___	NaCl_____	MgSO4.6H2O___	KMgClSO4.3H2O	KHCO3_____	MgSO4.H2O____
163	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
164	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*
165	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
166	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
167	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
168	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
169	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
170	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
171	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
172	10)	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	*0.00000E+00*	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

Appendix R: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

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	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	K2Mg(SO4)2.4H	Na4Ca(SO4)3.2	MgCO3_____	Mg2Cl(OH)3.4H	KHSO4_____	Na2SO4.10H2O_	K8H6(SO4)7___	NaHCO3_____	Na2CO3.10H2O_
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	MgCO3.3H2O___	K2Mg(SO4)2.6H	Na2Ca(CO3)2.2	K2MgCa2(SO4)4	Ca(OH)2_____	K2CO3.3/2H2O_	K8H4(CO3)6.3H	KNaCO3.6H2O__	K2NaH(CO3)2.2
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	K3H(SO4)2__Se	Na3H(SO4)2___	Na2CO3.7H2O__	KCl_____	K2Ca(SO4)2.H2	Mg2CaCl6.12H2	Na2SO4_____	Na2CO3.H2O___	Na3H(CO3)2.2H
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	Na2B4O7.10H2O	B(OH)3_____	KB5O8.4H2O___	K2B4O7.4H2O__	NaBO2.4H2O___	NaB5O8.5H2O__	NaBO2.NaCl.2H
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

	IonicStreng	Eh[=]Volts	TitrVol,ml	pH
1)	5.61119E+00	0.00000E+00	0.00000E+00	5.3205
2)	5.61031E+00	0.00000E+00	0.10000	5.6451
3)	5.61008E+00	0.00000E+00	0.14251	5.9936
4)	5.61006E+00	0.00000E+00	0.20309	7.9427
5)	5.61049E+00	0.00000E+00	0.28943	8.8722
6)	5.61112E+00	0.00000E+00	0.41246	9.2225
7)	5.61202E+00	0.00000E+00	0.58780	9.4695
8)	5.61330E+00	0.00000E+00	0.83768	9.6719
9)	5.61513E+00	0.00000E+00	1.1938	9.8493
10)	5.61774E+00	0.00000E+00	1.7013	10.010
11)	5.62149E+00	0.00000E+00	2.4245	10.158
12)	5.62685E+00	0.00000E+00	3.4551	10.295
13)	5.63455E+00	0.00000E+00	4.9239	10.424
14)	5.64559E+00	0.00000E+00	7.0170	10.545
15)	5.66143E+00	0.00000E+00	10.000	10.659

Appendix S: Sample Output File "Np_NaCl_BM_LIN.TITRATE"

```
Benchmark TITRATE Problem, LINEAR option; Np(V)O2 with CO3 in 5.61molal NaCl  FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

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, molal


      H2O           Na+           K+            Ca++          Mg++          MgOH+         H+            Cl-           SO4=
 1)  1.92928E+01  5.61057E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.21872E-06  5.61096E+00  0.00000E+00
 2)  1.92978E+01  5.61014E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.77346E-07  5.60993E+00  0.00000E+00
 3)  1.93027E+01  5.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.87609E-09  5.60892E+00  0.00000E+00
 4)  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
 5)  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
 6)  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
 7)  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
 8)  1.93277E+01  5.61001E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  6.82959E-11  5.60375E+00  0.00000E+00
 9)  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
10)  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
11)  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
12)  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
13)  1.93527E+01  5.61002E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.60509E-11  5.59859E+00  0.00000E+00
14)  1.93577E+01  5.61002E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.30838E-11  5.59756E+00  0.00000E+00
15)  1.93627E+01  5.61002E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.06048E-11  5.59653E+00  0.00000E+00

      HSO4-         OH-           HCO3-         CO3=          CO2(aq)       CaCO3(aq)     MgCO3(aq)     B(OH)3(aq)    B(OH)4-
 1)  0.00000E+00  3.01685E-09  2.26571E-04  3.09384E-08  3.86103E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 2)  0.00000E+00  6.37029E-09  3.82212E-04  1.10196E-07  3.08476E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 3)  0.00000E+00  9.49137E-07  9.89705E-04  4.25167E-05  5.36072E-06  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
 4)  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
 5)  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
 6)  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
 7)  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
 8)  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
 9)  0.00000E+00  6.40010E-05  1.06176E-03  3.07597E-03  8.51877E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
10)  0.00000E+00  7.38545E-05  1.07138E-03  3.58175E-03  7.44762E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
11)  0.00000E+00  8.35411E-05  1.08082E-03  4.08730E-03  6.64082E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
12)  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
13)  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
14)  0.00000E+00  1.11676E-04  1.10821E-03  5.60253E-03  5.09071E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
15)  0.00000E+00  1.20768E-04  1.11706E-03  6.10711E-03  4.74407E-08  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

        (missing species have zero amounts)

      NpO2+         NpO2OH(aq)    NpO2(OH)2-    NpO2CO3-      NpO2(CO3)2=-  NpO2(CO3)3==- Am+++         AmCO3+        Am(CO3)2-
 1)  6.12705E-04  7.72186E-10  2.04381E-16  1.33526E-07  1.98384E-11  1.25197E-16  0.00000E+00  0.00000E+00  0.00000E+00
 2)  1.72085E-04  4.57851E-10  2.55903E-16  1.33573E-07  7.06677E-11  1.58546E-15  0.00000E+00  0.00000E+00  0.00000E+00
 3)  4.46247E-07  1.76865E-10  1.47303E-14  1.33612E-07  2.72677E-08  2.35800E-10  0.00000E+00  0.00000E+00  0.00000E+00
 4)  3.48770E-08  1.73300E-10  1.81034E-13  1.33632E-07  3.48878E-07  3.85776E-08  0.00000E+00  0.00000E+00  0.00000E+00
 5)  1.80727E-08  1.71468E-10  3.42173E-13  1.33651E-07  6.73247E-07  1.43575E-07  0.00000E+00  0.00000E+00  0.00000E+00
 6)  1.22005E-08  1.69754E-10  4.97012E-13  1.33671E-07  9.97249E-07  3.14830E-07  0.00000E+00  0.00000E+00  0.00000E+00
 7)  9.21138E-09  1.68120E-10  6.45975E-13  1.33690E-07  1.32081E-06  5.51937E-07  0.00000E+00  0.00000E+00  0.00000E+00
 8)  7.40067E-09  1.66553E-10  7.89467E-13  1.33710E-07  1.64391E-06  8.54484E-07  0.00000E+00  0.00000E+00  0.00000E+00
 9)  6.18630E-09  1.65046E-10  9.27855E-13  1.33729E-07  1.96653E-06  1.22205E-06  0.00000E+00  0.00000E+00  0.00000E+00
10)  5.31533E-09  1.63595E-10  1.06147E-12  1.33749E-07  2.28868E-06  1.65423E-06  0.00000E+00  0.00000E+00  0.00000E+00
11)  4.66017E-09  1.62195E-10  1.19063E-12  1.33768E-07  2.61033E-06  2.15059E-06  0.00000E+00  0.00000E+00  0.00000E+00
12)  4.14945E-09  1.60844E-10  1.31559E-12  1.33788E-07  2.93150E-06  2.71072E-06  0.00000E+00  0.00000E+00  0.00000E+00
13)  3.74015E-09  1.59537E-10  1.43661E-12  1.33807E-07  3.25216E-06  3.33418E-06  0.00000E+00  0.00000E+00  0.00000E+00
14)  3.40480E-09  1.58274E-10  1.55392E-12  1.33827E-07  3.57233E-06  4.02056E-06  0.00000E+00  0.00000E+00  0.00000E+00
15)  3.12502E-09  1.57050E-10  1.66773E-12  1.33846E-07  3.89199E-06  4.76942E-06  0.00000E+00  0.00000E+00  0.00000E+00

      Am(CO3)3=-    Am(OH)2+      Am(OH)3(aq)   Th++++        UO2++         NpO2OH(aged)_ NpO2OH(amor)_ NaNpO2CO3(s)_ Na3NpO2(CO3)2
 1)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99932E+00  0.00000E+00
 2)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99718E+00  0.00000E+00
 3)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99481E+00  0.00000E+00
 4)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.99222E+00  0.00000E+00
 5)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.98964E+00  0.00000E+00
 6)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.98705E+00  0.00000E+00
 7)  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.98446E+00  0.00000E+00
```

Appendix S: Sample Output File "Np_NaCl_BM_LIN.TITRATE"

8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98188E+00	0.00000E+00
9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97930E+00	0.00000E+00
10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97672E+00	0.00000E+00
11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97413E+00	0.00000E+00
12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97156E+00	0.00000E+00
13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96898E+00	0.00000E+00
14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96640E+00	0.00000E+00
15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96382E+00	0.00000E+00

(missing species have zero amounts)

	IonicStreng	Eh[=]Volts	TitrVol,ml	pH
1)	5.61119E+00	0.00000E+00	0.00000E+00	5.3205
2)	5.61031E+00	0.00000E+00	0.10000	5.6451
3)	5.61004E+00	0.00000E+00	0.20000	7.8183
4)	5.61055E+00	0.00000E+00	0.30000	8.9167
5)	5.61106E+00	0.00000E+00	0.40000	9.1977
6)	5.61157E+00	0.00000E+00	0.50000	9.3641
7)	5.61208E+00	0.00000E+00	0.60000	9.4821
8)	5.61259E+00	0.00000E+00	0.70000	9.5733
9)	5.61310E+00	0.00000E+00	0.80000	9.6473
10)	5.61362E+00	0.00000E+00	0.90000	9.7095
11)	5.61413E+00	0.00000E+00	1.0000	9.7631
12)	5.61464E+00	0.00000E+00	1.1000	9.8100
13)	5.61516E+00	0.00000E+00	1.2000	9.8517
14)	5.61567E+00	0.00000E+00	1.3000	9.8892
15)	5.61619E+00	0.00000E+00	1.4000	9.9232

Appendix T: Sample Output File "Np_NaCl_BM.TITRATE"

```
Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl                FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31   Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,F91,RFFR92,RFF94,RRFF94)

Titrant Volumes per Grid Block, in milliliters
  1            0.000000 mL
  2            0.100000 mL
  3            0.142510 mL
  4            0.160000 mL
  5            0.180000 mL
  6            0.203090 mL
  7            0.220000 mL
  8            0.240000 mL
  9            0.260000 mL
 10            0.289430 mL
 11            0.412460 mL
 12            0.587800 mL
 13            1.193800 mL
 14            3.455100 mL
 15           10.000000 mL


Titration Results, molal

```

	H2O	Na+	K+	Ca++	Mg++	MgOH+	H+	Cl-	SO4=
1)	1.92928E+01	5.61057E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.21872E-06	5.61096E+00	0.00000E+00
2)	1.92978E+01	5.61014E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.77346E-07	5.60993E+00	0.00000E+00
3)	1.92999E+01	5.61003E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.58815E-07	5.60950E+00	0.00000E+00
4)	1.93007E+01	5.61001E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.48381E-07	5.60933E+00	0.00000E+00
5)	1.93017E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.09374E-08	5.60913E+00	0.00000E+00
6)	1.93029E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.91107E-09	5.60889E+00	0.00000E+00
7)	1.93037E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.18855E-09	5.60872E+00	0.00000E+00
8)	1.93047E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	6.93877E-10	5.60851E+00	0.00000E+00
9)	1.93057E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.89995E-10	5.60830E+00	0.00000E+00
10)	1.93072E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.42501E-10	5.60800E+00	0.00000E+00
11)	1.93133E+01	5.61000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.52981E-10	5.60673E+00	0.00000E+00
12)	1.93221E+01	5.61001E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.66958E-11	5.60491E+00	0.00000E+00
13)	1.93524E+01	5.61002E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.62542E-11	5.59866E+00	0.00000E+00
14)	1.94655E+01	5.61007E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.31074E-11	5.57548E+00	0.00000E+00
15)	1.97930E+01	5.61035E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.83272E-12	5.50989E+00	0.00000E+00

	HSO4-	OH-	HCO3-	CO3=	CO2(aq)	CaCO3(aq)	MgCO3(aq)	B(OH)3(aq)	B(OH)4-
1)	0.00000E+00	3.01685E-09	2.26571E-04	3.09384E-08	3.86103E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2)	0.00000E+00	6.37029E-09	3.82212E-04	1.10196E-07	3.08476E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3)	0.00000E+00	1.42122E-08	5.79854E-04	3.72976E-07	2.09764E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4)	0.00000E+00	2.47909E-08	7.06447E-04	7.92644E-07	1.46506E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5)	0.00000E+00	7.22202E-08	8.74979E-04	2.86004E-06	6.22872E-05	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6)	0.00000E+00	1.26379E-06	9.92658E-04	5.67805E-05	4.03803E-06	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7)	0.00000E+00	3.09556E-06	9.99205E-04	1.39997E-04	1.65938E-06	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8)	0.00000E+00	5.30281E-06	1.00274E-03	2.40670E-04	9.72059E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9)	0.00000E+00	7.50984E-06	1.00546E-03	3.41763E-04	6.88224E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10)	0.00000E+00	1.07451E-05	1.00903E-03	4.90734E-04	4.82685E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11)	0.00000E+00	2.40681E-05	1.02256E-03	1.11397E-03	2.18331E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12)	0.00000E+00	4.24987E-05	1.04073E-03	2.00200E-03	1.25799E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13)	0.00000E+00	1.01868E-04	1.09867E-03	5.06639E-03	5.53395E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14)	0.00000E+00	2.84255E-04	1.27533E-03	1.64154E-02	2.29199E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15)	0.00000E+00	6.55397E-04	1.63010E-03	4.83971E-02	1.25492E-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

(missing species have zero amounts)

	NpO2+	NpO2OH(aq)	NpO2(OH)2-	NpO2CO3-	NpO2(CO3)2=-	NpO2(CO3)3===	Am+++	AmCO3+	Am(CO3)2-
1)	6.12705E-04	7.72186E-10	2.04381E-16	1.33526E-07	1.98384E-11	1.25197E-16	0.00000E+00	0.00000E+00	0.00000E+00
2)	1.72085E-04	4.57851E-10	2.55903E-16	1.33573E-07	7.06677E-11	1.58546E-15	0.00000E+00	0.00000E+00	0.00000E+00
3)	5.08524E-05	3.01827E-10	3.76382E-16	1.33591E-07	2.39199E-10	1.81536E-14	0.00000E+00	0.00000E+00	0.00000E+00
4)	2.39307E-05	2.47753E-10	5.38926E-16	1.33598E-07	5.08355E-10	8.19789E-14	0.00000E+00	0.00000E+00	0.00000E+00
5)	6.63303E-06	2.00045E-10	1.26769E-15	1.33606E-07	1.83431E-09	1.06720E-12	0.00000E+00	0.00000E+00	0.00000E+00
6)	3.34150E-07	1.76340E-10	1.95555E-14	1.33613E-07	3.64151E-08	4.20537E-10	0.00000E+00	0.00000E+00	0.00000E+00
7)	1.35537E-07	1.75190E-10	4.75887E-14	1.33616E-07	8.97771E-08	2.55580E-09	0.00000E+00	0.00000E+00	0.00000E+00
8)	7.88495E-08	1.74579E-10	8.12402E-14	1.33620E-07	1.54320E-07	7.55070E-09	0.00000E+00	0.00000E+00	0.00000E+00
9)	5.55313E-08	1.74113E-10	1.14749E-13	1.33624E-07	2.19119E-07	1.52213E-08	0.00000E+00	0.00000E+00	0.00000E+00
10)	3.86794E-08	1.73507E-10	1.63619E-13	1.33630E-07	3.14582E-07	3.13678E-08	0.00000E+00	0.00000E+00	0.00000E+00
11)	1.70496E-08	1.71249E-10	3.61801E-13	1.33654E-07	7.13640E-07	1.61308E-07	0.00000E+00	0.00000E+00	0.00000E+00
12)	9.49502E-09	1.68316E-10	6.28103E-13	1.33688E-07	1.28136E-06	5.19497E-07	0.00000E+00	0.00000E+00	0.00000E+00
13)	3.76315E-09	1.59617E-10	1.42922E-12	1.33806E-07	3.23230E-06	3.29369E-06	0.00000E+00	0.00000E+00	0.00000E+00
14)	1.17432E-09	1.38078E-10	3.46327E-12	1.34242E-07	1.03462E-05	3.32871E-05	0.00000E+00	0.00000E+00	0.00000E+00
15)	4.11022E-10	1.09291E-10	6.38945E-12	1.35468E-07	2.94209E-05	2.58546E-04	0.00000E+00	0.00000E+00	0.00000E+00

	Am(CO3)3=-	Am(OH)2+	Am(OH)3(aq)	Th++++	UO2++	NpO2OH(aged)_	NpO2OH(amor)_	NaNpO2CO3(s)_	Na3NpO2(CO3)2
1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99932E+00	0.00000E+00
2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99718E+00	0.00000E+00
3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99622E+00	0.00000E+00
4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99580E+00	0.00000E+00
5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99531E+00	0.00000E+00
6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99473E+00	0.00000E+00
7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99430E+00	0.00000E+00

Appendix T: Sample Output File "Np_NaCl_BM.TITRATE"

87	8)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99378E+00	0.00000E+00
88	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99326E+00	0.00000E+00
89	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.99250E+00	0.00000E+00
90	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98931E+00	0.00000E+00
91	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98478E+00	0.00000E+00
92	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.96914E+00	0.00000E+00
93	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.91117E+00	0.00000E+00
94	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.74696E+00	0.00000E+00
95										
96		(missing species have zero amounts)								
97										

		IonicStreng	Eh[=]Volts	TitrVol,ml	pH
99	1)	5.61119E+00	0.00000E+00	0.00000E+00	5.3205
100	2)	5.61031E+00	0.00000E+00	0.10000	5.6451
101	3)	5.61008E+00	0.00000E+00	0.14251	5.9936
102	4)	5.61003E+00	0.00000E+00	0.16000	6.2353
103	5)	5.61001E+00	0.00000E+00	0.18000	6.6996
104	6)	5.61006E+00	0.00000E+00	0.20309	7.9427
105	7)	5.61014E+00	0.00000E+00	0.22000	8.3317
106	8)	5.61024E+00	0.00000E+00	0.24000	8.5655
107	9)	5.61034E+00	0.00000E+00	0.26000	8.7166
108	10)	5.61049E+00	0.00000E+00	0.28943	8.8722
109	11)	5.61112E+00	0.00000E+00	0.41246	9.2225
110	12)	5.61202E+00	0.00000E+00	0.58780	9.4695
111	13)	5.61513E+00	0.00000E+00	1.1938	9.8493
112	14)	5.62685E+00	0.00000E+00	3.4551	10.295
113	15)	5.66143E+00	0.00000E+00	10.000	10.659

Appendix U: Sample Output File "Np_NaCl_BM_LOG.MOLES"

See Table 30 for explanation of this listing.

```
Benchmark TITRATE Problem, LOG10 option; Np(V)O2 with CO3 in 5.61molal NaCl   FMT V2.0
DATABASE:  HMW84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94);
95.01.31      Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

   INITIAL and INJECTED Abundances BEFORE Flashing
   Hydrogen       1.1101736300E+02    1.1101836300E+02
   Oxygen         6.1508681500E+01    1.0550868200E+02
   Sodium         5.6100000000E+00    1.5610000000E+01
   Potassium      0.0000000000E+00    0.0000000000E+00
   Magnesium      0.0000000000E+00    0.0000000000E+00
   Calcium        0.0000000000E+00    0.0000000000E+00
   Chlorine       1.6100000000E+00    5.6110000000E+00
   Sulfur         0.0000000000E+00    0.0000000000E+00
   Carbon         2.0000000100E+00    1.0000000000E+01
   PosIon         0.0000000000E+00    0.0000000000E+00
   NegIon         0.0000000000E+00    0.0000000000E+00
   Air            0.0000000000E+00    0.0000000000E+00
   Boron          0.0000000000E+00    0.0000000000E+00
   Bromine        0.0000000000E+00    0.0000000000E+00
   TracerEl       0.0000000000E+00    0.0000000000E+00
   Th(IV)         0.0000000000E+00    0.0000000000E+00
   Am(III)        0.0000000000E+00    0.0000000000E+00
   U(VI)          0.0000000000E+00    0.0000000000E+00
   Np(V)          0.0000000000E+00    1.0000000000E+01
   ClO4-(EL)      0.0000000000E+00    0.0000000000E+00
   Phosphorus     0.0000000000E+00    0.0000000000E+00
   Electron       0.0000000000E+00    0.0000000000E+00
   Charge        -2.2204460500E-15   -2.3731663200E-15

   INITIAL and INJECTED Abundances AFTER Flashing
   Hydrogen       1.1101736300E+02    1.1101836300E+02
   Oxygen         6.1508681520E+01    1.0550868150E+02
   Sodium         5.6100000000E+00    1.5610000000E+01
   Potassium      0.0000000000E+00    0.0000000000E+00
   Magnesium      0.0000000000E+00    0.0000000000E+00
   Calcium        0.0000000000E+00    0.0000000000E+00
   Chlorine       1.6100000000E+00    5.6110000000E+00
   Sulfur         0.0000000000E+00    0.0000000000E+00
   Carbon         2.0000000100E+00    1.0000000000E+01
   PosIon         0.0000000000E+00    0.0000000000E+00
   NegIon         0.0000000000E+00    0.0000000000E+00
   Air            0.0000000000E+00    0.0000000000E+00
   Boron          0.0000000000E+00    0.0000000000E+00
   Bromine        0.0000000000E+00    0.0000000000E+00
   TracerEl       0.0000000000E+00    0.0000000000E+00
   Th(IV)         0.0000000000E+00    0.0000000000E+00
   Am(III)        0.0000000000E+00    0.0000000000E+00
   U(VI)          0.0000000000E+00    0.0000000000E+00
   Np(V)          0.0000000000E+00    1.0000000000E+01
   ClO4-(EL)      0.0000000000E+00    0.0000000000E+00
   Phosphorus     0.0000000000E+00    0.0000000000E+00
   Electron       0.0000000000E+00    0.0000000000E+00
   Charge        -2.2204460493E-15   -2.3731663190E-15

   INITIAL and INJECTED Concs AFTER Flashing, molal
   H2O                          WATER  5.5502535E+01  5.5509068E+01
   Na+                            Na+  5.6100000E+00  5.6106128E+00
   K+                              K+  0.0000000E+00  0.0000000E+00
   Ca++                          Ca++  0.0000000E+00  0.0000000E+00
   Mg++                          Mg++  0.0000000E+00  0.0000000E+00
   MgOH+                        MgOH+  0.0000000E+00  0.0000000E+00
   H+                              H+  2.3992707E-12  1.2187250E-06
   Cl-                            Cl-  1.6100000E+00  5.6110000E+00
   SO4=                          SO4=  0.0000000E+00  0.0000000E+00
   HSO4-                        HSO4-  0.0000000E+00  0.0000000E+00
   OH-                            OH-  6.1466486E-03  3.0168704E-09
   HCO3-                        HCO3-  6.1466639E-03  2.2657297E-04
   CO3=                          CO3=  1.9938533E+00  3.0938611E-08
   CO2(aq)                    CO2(aq)  2.3684969E-09  3.8610605E-04
   CaCO3(aq)                CaCO3(aq)  0.0000000E+00  0.0000000E+00
   MgCO3(aq)                MgCO3(aq)  0.0000000E+00  0.0000000E+00
   B(OH)3(aq)              B(OH)3(aq)  0.0000000E+00  0.0000000E+00
   B(OH)4-                   B(OH)4-  0.0000000E+00  0.0000000E+00
   B3O3(OH)4-              B3O3(OH)4-  0.0000000E+00  0.0000000E+00
   B4O5(OH)4=              B4O5(OH)4=  0.0000000E+00  0.0000000E+00
   CaB(OH)4+                CaB(OH)4+  0.0000000E+00  0.0000000E+00
   MgB(OH)4+                MgB(OH)4+  0.0000000E+00  0.0000000E+00
   Br-                            Br-  0.0000000E+00  0.0000000E+00
   ClO4-            perchlorate ClO4-  0.0000000E+00  0.0000000E+00
   NaOH(aq).....to.titrate.base.only   0.0000000E+00  0.0000000E+00
   HCl(aq).....to.titrate.acid.only    0.0000000E+00  0.0000000E+00
   HClO4(aq)....to.titrate.acid.only   0.0000000E+00  0.0000000E+00
```

Appendix U: Sample Output File "Np_NaCl_BM_LOG.MOLES"

```
PosIon.....POSITIVE.ION 0.0000000E+00 0.0000000E+00
NegIon.....NEGATIVE.ION 0.0000000E+00 0.0000000E+00
PosIon(OH)(aq).....to.titrate.base 0.0000000E+00 0.0000000E+00
HNegIon(aq).....to.titrate.acid 0.0000000E+00 0.0000000E+00
Tracer(aq).....conservative.tracer 0.0000000E+00 0.0000000E+00
H3PO4(aq) H3PO4(aq) 0.0000000E+00 0.0000000E+00
H2PO4- H2PO4- 0.0000000E+00 0.0000000E+00
HPO4= HPO4= 0.0000000E+00 0.0000000E+00
PO4=- PO4=- 0.0000000E+00 0.0000000E+00
NpO2+ NpO2+ 0.0000000E+00 6.1270920E-04
NpO2OH(aq) NpO2OH(aq) 0.0000000E+00 7.7219130E-10
NpO2(OH)2- NpO2(OH)2- 0.0000000E+00 2.0438298E-16
NpO2CO3- NpO2CO3- 0.0000000E+00 1.3352733E-07
NpO2(CO3)2=- NpO2(CO3)2=- 0.0000000E+00 1.9838516E-11
NpO2(CO3)3=-- NpO2(CO3)3=-- 0.0000000E+00 1.2519757E-16
Am+++ Am+++ 0.0000000E+00 0.0000000E+00
AmCO3+ AmCO3+ 0.0000000E+00 0.0000000E+00
Am(CO3)2- Am(CO3)2- 0.0000000E+00 0.0000000E+00
Am(CO3)3=- Am(CO3)3=- 0.0000000E+00 0.0000000E+00
Am(OH)2+ Am(OH)2+ 0.0000000E+00 0.0000000E+00
Am(OH)3(aq) Am(OH)3(aq) 0.0000000E+00 0.0000000E+00
Th++++ Th++++ 0.0000000E+00 0.0000000E+00
UO2++ U(VI)O2++ 0.0000000E+00 0.0000000E+00
NpO2OH(aged)_____NpO2OH(aged) 0.0000000E+00 0.0000000E+00
NpO2OH(amor)_____NpO2OH(amor) 0.0000000E+00 0.0000000E+00
NaNpO2CO3(s)_____NaNpO2CO3(s) 0.0000000E+00 9.9993872E+00
Na3NpO2(CO3)2(s)_DISABLED_DISABLED 0.0000000E+00 0.0000000E+00
AmOHCO3(c)_____AmOHCO3(c) 0.0000000E+00 0.0000000E+00
Am(OH)3(s)_____Am(OH)3(s) 0.0000000E+00 0.0000000E+00
NaAm(CO3)2.6H2O(c)_____ 0.0000000E+00 0.0000000E+00
AmPO4(c)_____AmPO4(c) 0.0000000E+00 0.0000000E+00
CaSO4_____Anhydrite 0.0000000E+00 0.0000000E+00
NaK3(SO4)2__Aphthitalite/Glaserite 0.0000000E+00 0.0000000E+00
CaCl2.6H2O_____Antarcticite 0.0000000E+00 0.0000000E+00
CaCO3_____Aragonite 0.0000000E+00 0.0000000E+00
K2SO4_____Arcanite 0.0000000E+00 0.0000000E+00
MgCl2.6H2O_____Bischofite 0.0000000E+00 0.0000000E+00
Na2Mg(SO4)2.4H2O_____Bloedite 0.0000000E+00 0.0000000E+00
Mg(OH)2_____Brucite 0.0000000E+00 0.0000000E+00
Na6CO3(SO4)2_____Burkeite 0.0000000E+00 0.0000000E+00
CaCO3_____Calcite 0.0000000E+00 0.0000000E+00
CaCl2.4H2O_____CaCl2_Tetrahydrite 0.0000000E+00 0.0000000E+00
Ca4Cl2(OH)6.13H2O__CaOxychloride A 0.0000000E+00 0.0000000E+00
Ca2Cl2(OH)2.H2O____CaOxychloride B 0.0000000E+00 0.0000000E+00
KMgCl3.6H2O_____Carnallite 0.0000000E+00 0.0000000E+00
MgSO4.7H2O_____Epsomite 0.0000000E+00 0.0000000E+00
CaNa2(CO3)2.5H2O_____Gaylussite 0.0000000E+00 0.0000000E+00
Na2Ca(SO4)2_____Glauberite 0.0000000E+00 0.0000000E+00
CaSO4.2H2O_____Gypsum 0.0000000E+00 0.0000000E+00
NaCl_____Halite 0.0000000E+00 0.0000000E+00
MgSO4.6H2O_____Hexahydrite 0.0000000E+00 0.0000000E+00
KMgClSO4.3H2O_____Kainite 0.0000000E+00 0.0000000E+00
KHCO3_____Kalicinite 0.0000000E+00 0.0000000E+00
MgSO4.H2O_____ Kieserite 0.0000000E+00 0.0000000E+00
K2Mg(SO4)2.4H2O_____Leonite 0.0000000E+00 0.0000000E+00
Na4Ca(SO4)3.2H2O_____Labile_Salt 0.0000000E+00 0.0000000E+00
MgCO3_____Magnesite 0.0000000E+00 0.0000000E+00
Mg2Cl(OH)3.4H2O_____MgOxychloride 0.0000000E+00 0.0000000E+00
KHSO4_____Mercallite 0.0000000E+00 0.0000000E+00
Na2SO4.10H2O_____Mirabilite 0.0000000E+00 0.0000000E+00
K8H6(SO4)7_____Misenite 0.0000000E+00 0.0000000E+00
NaHCO3_____Nahcolite 0.0000000E+00 0.0000000E+00
Na2CO3.10H2O_____Natron 0.0000000E+00 0.0000000E+00
MgCO3.3H2O_____Nesquehonite 0.0000000E+00 0.0000000E+00
K2Mg(SO4)2.6H2O Picromerite/Schoen 0.0000000E+00 0.0000000E+00
Na2Ca(CO3)2.2H2O_____Pirssonite 0.0000000E+00 0.0000000E+00
K2MgCa2(SO4)4.2H2O_____Polyhalite 0.0000000E+00 0.0000000E+00
Ca(OH)2_____Portlandite 0.0000000E+00 0.0000000E+00
K2CO3.3/2H2O___Potassium_Carbonate 0.0000000E+00 0.0000000E+00
K8H4(CO3)6.3H2O___K-Sequicarbonate 0.0000000E+00 0.0000000E+00
KNaCO3.6H2O_____K-Na-Carbonate 0.0000000E+00 0.0000000E+00
K2NaH(CO3)2.2H2O___Potassium_Trona 0.0000000E+00 0.0000000E+00
K3H(SO4)2__Sesquipotassium_Sulfate 0.0000000E+00 0.0000000E+00
Na3H(SO4)2____Sesquisodium_Sulfate 0.0000000E+00 0.0000000E+00
Na2CO3.7H2O____Na2CO3-Heptahydrate 0.0000000E+00 0.0000000E+00
KCl_____Sylvite 0.0000000E+00 0.0000000E+00
K2Ca(SO4)2.H2O_____Syngenite 0.0000000E+00 0.0000000E+00
Mg2CaCl6.12H2O_____Tachyhydrite 0.0000000E+00 0.0000000E+00
Na2SO4_____Thenardite 0.0000000E+00 0.0000000E+00
Na2CO3.H2O_____Thermonatrite 0.0000000E+00 0.0000000E+00
Na3H(CO3)2.2H2O_____Trona 0.0000000E+00 0.0000000E+00
Na2B4O7.10H2O_____ Borax 0.0000000E+00 0.0000000E+00
B(OH)3_____Borix_Acid_Solid 0.0000000E+00 0.0000000E+00
KB5O8.4H2O____K-Pentaborate_(30_C) 0.0000000E+00 0.0000000E+00
K2B4O7.4H2O___K-Tetraborate_(30_C) 0.0000000E+00 0.0000000E+00
NaBO2.4H2O_____Sodium_Metaborate 0.0000000E+00 0.0000000E+00
NaB5O8.5H2O_____Sodium_Pentaborate 0.0000000E+00 0.0000000E+00
NaBO2.NaCl.2H2O___Teepleite_(20_C) 0.0000000E+00 0.0000000E+00
```

Appendix V: Command File FMT_FMTC.COM

```
$   SET noverify
$!   SET verify
$!        FMT_FMTC.COM assigns and fetches user-selected
$!        chemdat and rhomin data base file names,
$!        assign user-specified input/output file names,
$!        executes fmt2p0 in CMS 1996 nonPA (Performance
$!        Asssessment) production area
$!
$!         Author:   K. M. Aragon
$!         Date:     11/17/95
$!
$!         Modifier: S. C. Babb
$!         Date:     12/13/95
$!
$!         Modifier: S. C. Babb
$!         Date:     12/18/95
$!         Reason:    use fmt executable in production area
$!                    print identity of fmt executable
$!                    add log file and mail facility
$!                    decided not to use mail facility
$!
$!         Modifier: S. C. Babb
$!         Date:     12/21/95
$!         Reason:   name of fmt executable changed to prefix
$!                   "fmt_" full name is fmt_fmt2p0_pa96.exe
$!
$!*****************************************************************************
$!  INPUTS:
$!
$!     P1 - Substring chemdat file name search on valance states, dates,
$!              and/or fugacity
$!
$!     P2 - Substring rhomin file name search on valance states and/or dates
$!
$!     P3 - Input File Name (no extension)
$!
$!-----------------------------------------------------------------------------
$!
$! Turn on error handling; exit on any error.
$!
$   ON error then goto error_exit
$   mode = f$mode()
$!
$! Logic flow
$!
$   GOSUB check_filename
$   GOSUB define_cms_library
$   GOSUB delete_files
$   GOSUB get_database_files
$   GOSUB define_inputs
$   GOSUB define_outputs
$   GOSUB start_log
$!   GOSUB start_mail
$   GOSUB run_fmt
$   GOSUB undefine_symbols
$   goto  terminate
$   EXIT
$!-----------------------------------------------------------------------------
$CHECK_FILENAME:
$! Determine if any or all file names are passed as parameters. If not,
$! prompt for one if this is an interactive session;
$! otherwise flag an error and exit
$!
$!  Check for P1 - this is the CHEMDAT name field
$!
$  IF mode .eqs. "BATCH" .and. p1 .eqs. ""
$  THEN
$      WRITE sys$output -
      "Can not run in batch without a chemdat file name (P1). exiting."
$      GOTO error_exit
$  ENDIF
$!
$!
$  IF p1 .eqs. ""
$   THEN
$       INQUIRE chemdat_name  -
                "Enter chemdat file name to search on"
$       IF chemdat_name .eqs. "" THEN goto error_exit
$  ELSE
$       chemdat_name = p1
$  ENDIF
$!
$!  Check for P2 - this is the RHOMIN name field
$!
$  IF mode .eqs. "BATCH" .and. p2 .eqs. ""
$  THEN
```

Appendix V: Command File FMT_FMTC.COM

```
$       WRITE sys$output -
       "Can not run in batch without a rhomin file name (P2). exiting."
$       GOTO error_exit
$  ENDIF
$!
$!
$  IF p2 .eqs. ""
$   THEN
$       INQUIRE rhomin_name  -
                "Enter rhomin file name to search on"
$       IF rhomin_name .eqs. "" THEN goto error_exit
$   ELSE
$       rhomin_name = p2
$   ENDIF
$!
$!  Check for P3 - this is the file name field
$!
$  IF mode .eqs. "BATCH" .and. p3 .eqs. ""
$  THEN
$      WRITE sys$output -
       "Can not run in batch without a file name (P3). exiting."
$      GOTO error_exit
$  ENDIF
$!
$!
$  IF p3 .eqs. ""
$   THEN
$       INQUIRE file_name  "Enter input file name (without .extension)"
$       IF file_name .eqs. "" THEN goto error_exit
$  ELSE
$       file_name = p3
$  ENDIF
$   RETURN
$!-----------------------------------------------------------------------------
$DEFINE_CMS_LIBRARY:
$! Define non-pa cms symbols and point to fmt library
$!
$!  set noverify
$  nonpa_cms_syms
$!
$! Set CMS library to FMT
$!
$   cms_library_name = "fmt"
$   lib'cms_library_name
$!  set verify
$!
$   RETURN
$!-----------------------------------------------------------------------------
$DEFINE_INPUTS:
$! Define the input files needed.
$!
$   DEFINE input 'file_name'.in
$   DEFINE inguess 'file_name'.inguess
$!
$! Define a logical that points to the database files just fetched
$!
$   DEFINE chemdat 'chemdat_name'
$   DEFINE rhomin 'rhomin_name'
$!
$   RETURN
$!-----------------------------------------------------------------------------
$DEFINE_OUTPUTS:
$! Define the output files needed.
$!
$   DEFINE output 'file_name'.out
$   DEFINE for088 'file_name'.for088
$   DEFINE titrate 'file_name'.titrate
$   DEFINE moles 'file_name'.moles
$!
$   RETURN
$!-----------------------------------------------------------------------------
$DELETE_FILES:
$!
$! Turn off warning messages for no files to delete
$!
$   SET noon
$   SET message/nofac/nosev/notext/noid
$! Delete all 'file_name'.moles files; do not accumulate them.
$!
$   DELETE  'file_name'.moles;*
$! Delete all fmt prefixed files of chemdat and rhomin files
$!
$   DELETE  fmt_*.chemdat;*
$   DELETE  fmt_*.rhomin;*
$   SET message/fac/sev/text/id
$   SET on
$!
$   RETURN
$!-----------------------------------------------------------------------------
$ERROR_EXIT:
```

Appendix V: Command File FMT_FMTC.COM

```
$! Exit routine when a severe error is encountered
$!
$   Write sys$output "Executing error exit, ''$status'."
$   EXIT
$!-------------------------------------------------------------------------------
$GET_DATABASE_FILES:
$!
$! If interactive, allow user to select/pick from a list of chemdat file names
$!
$  IF mode .nes. "BATCH"
$  THEN
$    cse "*''chemdat_name'*.chemdat"
$!
$    INQUIRE chemdat_name "Select CHEMDAT name from list above"
$  ENDIF
$!
$! Fetch chemdat from FMT CMS
$!
$!   set noverify
$   cfe 'chemdat_name'
$!  set verify
$!
$! If interactive allow user to select/pick from a list of rhomin file names
$!
$  IF mode .nes. "BATCH"
$  THEN
$    cse "*''rhomin_name'*.rhomin"
$!
$    INQUIRE rhomin_name "Select RHOMIN name from list above"
$  ENDIF
$!
$! Fetch chemdat from FMT CMS
$!   set noverify
$   cfe 'rhomin_name'
$!   set verify
$!
$   RETURN
$!-------------------------------------------------------------------------------
$RUN_FMT:
$! Define the run symbols needed.
$   define /nolog exe_dir               wp$nonpa_prodroot:[fmt.exe]
$   fmt2p0      :== *$exe_dir:fmt_fmt2p0_pa96.exe"
$!
$! Run the utility that shows image information from the exe. (mandatory!)
$! This is part of the documentation required while doing a calculation.
$   @wp$ref:wp_get_image_id.com         exe_dir:fmt_fmt2p0_pa96.exe
$! Run the code
$!
$   fmt2p0
$   RETURN
$!-------------------------------------------------------------------------------
$START_LOG:
$!
$   month   == f$cvtime("''f$time()'", "absolute", "month" )
$   day             == f$cvtime("''f$time()'", "comparison", "day" )
$   hour    == f$cvtime("''f$time()'", "absolute", "hour" )
$   min             == f$cvtime("''f$time()'", "absolute", "minute" )
$!
$   log_file_name :== "''file_name'_''month''day'_''hour''min'.log"
$!  mike williamson's log file definition:
$!      "sys$login:fmt_''file_name'_''month''day'_''hour''min'.log"
$!
$   DEFINE/proc sys$output 'log_file_name
$!
$   RETURN
$!-------------------------------------------------------------------------------
$START_MAIL:
$! Open a file where we can write a message that can be sent to the
$! user upon completion.
$!
$   mail_error_flag = 0
$   mail_file_name :== "sys$Login:fmt_mail.msg"
$   mail_subject   :== "FMT ''file_name' run."
$   mail_list == f$getjpi( "", "username")
$!
$   OPEN/write mail_file 'mail_file_name
$!
$   RETURN

$!-------------------------------------------------------------------------------
$TERMINATE:
$! If there was no previously flagged error or problem, search the log files
$! for any fatal, error, or warning messages.
$!
$! Deassign sys$output so the "log" file closes.
$   deassign sys$output
$!
$! Show the run output to the user
$   TYPE 'log_file_name
$!
```

Appendix V: Command File FMT_FMTC.COM

```
$! Skip sending the mail message
$   goto end_terminate
$!
$! If there was not a previous error recorded, search the log file for
$! common error indicators.
$   search_status = 0
$   IF mail_error_flag .ne. 1
$   THEN
$!      Turn off informational messages from search command
$       SET message/nofac/nosev/notext/noid
$       SEARCH 'log_file_name "-F-","-E-","-W-" / match=or
$       search_status = $status
$!      Turn on messages
$       SET message/fac/sev/text/id
$   ENDIF
$!
$   IF search_status .eq. 1 .or. mail_error_flag .eq. 1
$   THEN
$       WRITE mail_file  "The run log contains an error or warning. "
$       WRITE mail_file  "Please examine ''log_file_name'."
$       mail_subject    == "''mail_subject' ERROR"
$   ELSE
$       WRITE mail_file  "The FMT run has completed."
$   ENDIF
$!
$   CLOSE/nolog mail_file
$   MAIL/subject="''mail_subject'" 'mail_file_name 'mail_list
$!
$END_TERMINATE:
$   EXIT
$!-------------------------------------------------------------------------------
$UNDEFINE_SYMBOLS:
$! Deassign input files
$!
$   DEASSIGN input
$   DEASSIGN inguess
$   DEASSIGN chemdat
$   DEASSIGN rhomin
$   DEASSIGN output
$   DEASSIGN for088
$   DEASSIGN titrate
$   DEASSIGN moles
$!
$   RETURN
$!-------------------------------------------------------------------------------
$! CMS REPLACEMENT HISTORY, Element FMT_FMTC.COM
$! *2    21-DEC-1995 12:58:57 SCBABB "FMT EXECUTABLE NAME CHANGED"
$! *1    19-DEC-1995 12:26:54 SCBABB "USER COMMAND FILE FOR EXECUTING FMT_FMT2P0 FROM CMS"
$! CMS REPLACEMENT HISTORY, Element FMT_FMTC.COM
```

Appendix W: Review Forms

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