Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant

SOTERM Attachment 1



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WIPP PA

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User's Manual

for

FMT, Version 2.0

Document Version 1.00

WPO # 28119

,

November 17, 1995

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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 CO₂ 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.

$$\frac{\partial G}{\partial \bar{\xi}} = \mathbf{0}.$$
 (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, $\mathbf{N} = (\vec{v}_1, \vec{v}_2, ..., \vec{v}_R)$; entry (i,j) of N is v_{ij} , and

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

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

$$\delta\xi_{j}^{(m)} = -\left(\frac{\partial G}{\partial \xi_{j}}\right)^{(m)} = -\Delta G_{j}^{(m)}$$

$$= -\sum_{i=1}^{N'} v_{ij} \mu_{i}^{(m)}; \qquad j = 1, 2, \dots R ,$$
(3)

where

m = iteration index,

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

- N' = number of species excluding inert species,
- μ_i = chemical potential of species *i*, and

R = maximum number of linearly independent chemical equations.

The mole numbers are adjusted by means of



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

where n_i = the number of moles of species *i*.

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

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

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

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

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

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

where

R = the gas constant, 8.3143 J mole⁻¹ K⁻¹,

T = absolute temperature (K)

$$\delta_{kl}$$
 = 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

 $n_t = \text{total number of moles.}$

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

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

where \overline{v}_i is the sum of the stoichiometric coefficients in stoichiometric equation *i.*, i.e. $\overline{v}_i = \sum_{k=1}^{N'} v_{ki}$

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

$$\delta\xi_{j}^{(m)} = -\left(\frac{1}{n_{j+M}^{(m)}} + \sum_{k=1}^{M} \frac{\nu_{kj}^{2}}{n_{k}^{(m)}} - \frac{\overline{\nu}_{j}^{2}}{n_{l}}\right)^{-1} \frac{\Delta G_{j}^{(m)}}{RT}; \qquad j = 1, 2, \dots R$$
(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:



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

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

$$a_i = \gamma_i \mathbf{m}_i$$
 (A.1b)

and, for the solvent, by

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

where

 γ_i = the activity coefficient of the solute species,

 m_i = the molality of the solute species,

W = the molecular weight of water,

 $\sum_{i} m_{i}$ = the sum over all solutes (cations, anions, and 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:

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

The remaining variables lacking explicit definition are the excess functions γ_i and $(\phi-1)$. These functions, rewritten below, are modeled using the semiempirical equations of Pitzer (1973) and coworkers. (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.

~ *

$$(\phi-1) = \frac{2}{\left(\sum_{i} m_{i}\right)} \left\{ -\frac{A^{\phi}I^{3/2}}{1+bI^{1/2}} + \sum_{c} \sum_{a} m_{c}m_{a} \left(B_{ca}^{\phi} + ZC_{ca}\right) + \sum_{c} \sum_{c'} m_{c}m_{c'} \left(\Phi_{cc'}^{\phi} + \sum_{a} m_{a}\psi_{cc'a}\right) + \sum_{a} \sum_{a'} m_{a}m_{a'} \left(\Phi_{aa'}^{\phi} + \sum_{c} m_{c}\psi_{aa'c}\right) + \sum_{n} \sum_{c} m_{n}m_{c}\lambda_{nc}$$

$$+ \sum_{n} \sum_{a} m_{n}m_{a}\lambda_{na} + \sum_{n} \sum_{c} \sum_{a} m_{n}m_{c}m_{a}\zeta_{nca} \right\}$$

$$(A.2a)$$

$$\ln\gamma_{M} = z_{M}^{2}F + \sum_{a} m_{a} \left(2B_{Ma} + ZC_{Ma}\right) + \sum_{c} m_{c} \left(2\Phi_{Mc} + \sum_{a} m_{a} \Psi_{Mca}\right)$$

$$+ \sum_{a} \sum_{a'} m_{a} m_{a'} \Psi_{aa'M} + \left|z_{M}\right| \sum_{c} \sum_{a} m_{c} m_{a} C_{ca} + \sum_{n} m_{n} (2\lambda_{nM}) + \sum_{n} \sum_{a} m_{n} m_{a} \zeta_{naM}$$
(A.2b)

$$\ln\gamma_{X} = z_{M}^{2}F + \sum_{c} m_{c} \left(2B_{Xc} + ZC_{Xc}\right) + \sum_{a} m_{a} \left(2\Phi_{Xa} + \sum_{c} m_{c}\psi_{Xca}\right)$$

$$+ \sum_{c} \sum_{c'} m_{c} m_{c'}\psi_{cc'X} + \left|z_{X}\right| \sum_{c} \sum_{a} m_{c} m_{a}C_{ca} + \sum_{n} m_{n} \left(2\lambda_{nX}\right) + \sum_{n} \sum_{c} m_{n} m_{c}\zeta_{ncX}$$
(A.2c)

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

$$F = -A^{\phi} \left(\frac{I^{1/2}}{1 + bI^{1/2}} + \frac{2}{b} \ln(1 + bI^{1/2}) \right) + \sum_{c} \sum_{a} m_{c} m_{a} B'_{ca}$$
(A.2e)
+
$$\sum_{c} \sum_{c'} m_{c} m_{c'} \Phi'_{cc'} + \sum_{a} \sum_{a'} m_{a} m_{a'} \Phi'_{aa'}$$
(A.2e)
$$C_{MX} = \frac{C^{\phi}_{MX}}{2|Z_{M}Z_{X}|^{1/2}}$$
(2b)

. . .

$$Z = \sum_{i} |z_i| \mathbf{m}_i \tag{2c}$$

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

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

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

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

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

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

The functions g and g' are defined by

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

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

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

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

$$\Phi_{ij}^{\prime} = {}^{\mathsf{E}} \Theta_{ij}^{\prime}(\mathbf{I}) \tag{5c}$$

The functions ${}^{E}\theta_{ii}(I)$ and ${}^{E}\theta'_{ii}(I)$ 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_{ii} for each cation-cation and anion-anion pair
- Ψ_{ijk} for each cation-cation-anion and anion-anion-cation triplet
- λ_{ni} and ζ_{nii} for ion-neutral and ion-ion-neutral interactions.

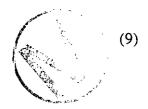
Many of these parameters can be assigned a value of zero. The above parameters are tabulated in the CHEMDAT data base (Section 7.3, Appendices I and J).

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:

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



and

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

ог

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

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

$$\mu_{i} = \mu_{i}^{*} [T, P, \mathbf{n}^{*}, (T, P)] + RT \ln x_{i}$$
(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 $\bar{\gamma}$ for the nonideal system are computed from a known chemical potential expression at the $\mathbf{n}^{(1)}$ composition. In the next step, the equilibrium composition in the "ideal" system is computed from equation 11, with μ_i^* replaced by

$$\mu_i^{*(1)} = \mu_i^* + RT \ln \gamma_i (T, P, \mathbf{n}^{(1)}).$$
(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, ClO₄, 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)," "CIO4," 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 CO₂ gas present. It is therefore desirable to calculate the effects of CO₂ gas on the aqueous and solid chemistry in the disposal room, and in turn on dissolved actinide concentrations. While FMT cannot explicitly model the gas phase, it can model a system with constant CO₂ gas fugacity by proper declaration of a CO₂ solid phase, as discussed below.

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

$$\operatorname{CO}_2(g) \leftrightarrow \operatorname{CO}_2(\operatorname{"solid"}).$$
 (13)

At equilibrium, this reaction is described by the relationship

$$\frac{\mu_{\rm CO_2("solid")}^0}{RT} = \frac{\mu_{\rm CO_2(g)}^0}{RT} + \ln f_{\rm CO_2},$$
(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 H₂O within FMT, is calculated based on the extrinsic amount of water that can be formed from the specified element abundances. This is the technical definition for the abundance entries. In practice, it is convenient to specify about 1 kg of water (about 55.5 moles of O and 111.0 moles of H) to allow the abundances in the INPUT and INGUESS files to be looked at on a molal (or approximately, molar) basis. (A convenient way to put all species concentrations in the INGUESS file on a nearly exact molal basis is through use of the FOR088 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 H₂O" basis.)

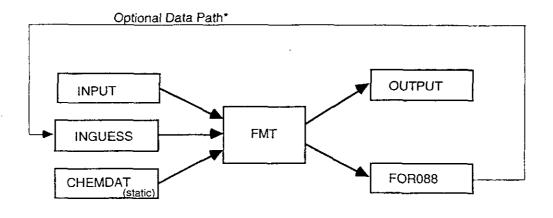
Optionally, the user could specify the same solution composition by setting the *species* abundances in the INGUESS file. The CHEMDAT file is a data base that contains species names, characteristics, and Pitzer parameters. RHOMIN, another data base file, contains mineral densities. FMT input files are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

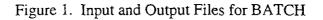
FMT generates a primary file OUTPUT and secondary file(s), depending on the problem. FOR088 is the secondary file for batch problems. TITRATE and MOLES are the secondary files for titrate problems. Both the FOR088 and TITRATE files are subsets of their respective OUTPUT files, reordered by chemical species 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.



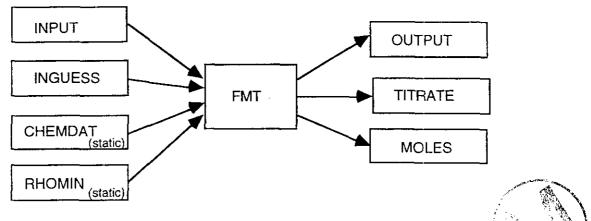


Figure 2. Input and Output Files for TITRATE

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_951213.CHEMDAT *LINTERACTIONS TO NP(V) SOLUBILITY W/O CMS HISTORY* FMT_HMW_35_951213_F-1.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-10.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-11.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-12.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-13.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-14.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-2.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-3.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-6.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-6.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-6.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-6.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-6.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-7.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-7.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-7.CHEMDAT *C02 FUGACITY FILES CREATED FROM FMT_HMW_35_951213.CHEMDAT MASTER FILE FROM CFNOVAK." FMT_HMW_35_951213_F-7.CHEMDAT *C02 F 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.REOMIN 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: "Al1-14" Entering Subroutine READDAT 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 DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-C1-ClO4 (NR94); 95.01.31 Am(III)-Na-C1-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94) FMT V2.0 Accuracy of reactions is Minimum elemental abundance is Number of Aqueous Species is 1,0000E-06 1.0000E-18 50 ACTIVITY COEF. FLAG PITZACT using PITZER ACTIVITY COEFFICIENT model Charge Balance replaces element Oxygen Exiting Subroutine READDAT Char Flags: FLOW/BATCH/TITRATE BATCH this is a BATCH problem UNUSED NEXACT Echo of Mole Specifications: nMOLES nE ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Hydrogen 55.1654821000000 0.200000000000000 Oxygen Sodium 0.1100000000000000 Chlorine 0.000000000000000000E+000 Posion 0.00000000000000E+000 Th(IV) 0.000000000000000E+000 Am(III) 0.000000000000000E+000 U(VI) 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)6.13H20_Ca0xychloride A; delaswitch *****************SOLUBILITY PRODUCT VIOLATION********* ____Brucite ** 1.00E+01 ** ** Mg (OH) 2___ ____ ** Mg2Cl(OH)3.4H20____MgOxychloride ** 6.69E+00 ** 2 Solubility Product Violations Adding solid Mg(OH)2pmH = -log[m(H+)]pH = -log[a(H+)]Total Diagonal Inversions85 _Brucite 12.7140

Total Stoichiometric Reoptimizations 10 SINGLE BATCH EQUILIBRATION COMPLETED S dir Directory U1: [SCBABB.FMT.CMS_TESTFILES] BATCH_DOC.FOR088;1 BATCH_DOC.IN;1 BATCH_DOC_JAN08_1519.LOG;1 BATCH_DOC.INGUESS;1 BATCH_DOC.OUT;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: "All-14" Entering Subroutine READDAT Entering Subjorting READBAT
reading chemical species data from CHEMDAT file
DG_BYPASS flag set to nDG_BYPASS
[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs
DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-Cl-Cl04 (NR94);
95.01.31 Am(III)-Na-Cl-CO3-S04-P04 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94) FMT V2.0 Accuracy of reactions is 1.0000E-06 Minimum elemental abundance is Number of Aqueous Species is 1.0000E-18 50 ACTIVITY COEF. FLAG PITZACT using PITZER ACTIVITY COEFFICIENT model Charge Balance replaces element Oxygen Exiting Subroutine READDAT Char Flags: FLOW/BATCH/TITRATE BATCH this is a BATCH problem INUSED Echo of Mole Specifications: nMOLES nE2 ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Hydrogen NEXACT Oxygen Sodium 1.000000000000000E-002 Potassium 1.000000000000000E-003 Magnesium 1.00000000000000E-004 Calcium 0.110000000000000 Chlorine 0.00000000000000E+000 NegIon 0.000000000000000E+000 Air 1.000000000000000E+000 Air 0.00000000000000E+000 Brown 0.00000000000000E+000 Brownine 0.000000000000000E+000 TracerEl 0.00000000000000E+000 Th(IV) 0.00000000000000E+000 Np(V) 0.000000000000000000E+000 Electron .LT. (MINABU*1.d-6) moles K8H4(CO3)6.3H20___K-Sequicarbonate; del&switch LT: (MINABU*1.d-6) moles B303(OH)4- B303(OH)4-; del&switch LT: (MINABU*1.d-6) moles Ca4Cl2(OH)6.13H2O_Ca0xychloride A; del&switch _Brucite ** 1.00E+01 ** ** Mg (OH) 2_ 2 Solubility Product Violations 2 Solubility Product Vio. Adding solid Mg(OH)2______ pmH = -log[m(H+)] pH = -log[a(H+)] = 12.8532 Total Diagonal Inversions ____Brucite 12.7140 85 Total Stoichiometric Reoptimizations SINGLE BATCH EQUILIBRATION COMPLETED 10

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.

FMT_HMW_NP_AM.RHOMIN:1

S địr

Directory U1: (SCBABB.FMT.CMS_TESTFILES)

FMT_HMW_NP_AM.CHEMDAT;1
NP_NACL_BM.INGUESS;2 FMT FMTC.COM:1 NP_NACL_BM.IN:5

Total of 5 files. S @fmt_fmtc Enter chemdat file name to search on: mp Enter rhomin file name to search on: mp Enter rhomin file name (without .extension): mp_macl_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: WPSNONPA_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: *All-14*

Entering Subroutine READDAT reading chemical species data from CHEMDAT file reading chemical species data from CHEMDAT file DG_BYPASS flag set to nDG_BYPASS Benchmark TITRATE Problem; Np(V)02 with C03 in 5.61molal NaCl DATABASE: HMW84/FW86; Np(V)-Na-C03-OH-Cl-Cl04 (NR94); 95.01.31 Am(III)-Na-Cl-C03-S04-P04 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94) FMT V2.0

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 Character Flags: I.C. nMOLES TEMP is an unused local variable nEXACT nEXACI 180000,10000000

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 Parameters FBAC ELO 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 Char Flags UNUSED UNUSED nMOLES LHSEDIE NEXACT



TEMP is an unused local variable 9.99 Character Flags: VPOROS FRFLASH VPOROS 9.99999999999999999E-021 FRFLASH Specifying VARIABLE POROSITY for TITRATION Problem Character Flags: VAR_AO_RHO VAR_AO_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" $pmH \neq -log[m(H+)]$ 11.6199 11.7497 pH = -log[a(H+)]pmH = -log[m(H+)]= 5.9141 pH = -log[a(H+)]5.3205 TITRATION Character Flags cduml= TITRATE cdum cdum2= ASREAD reading titrant volumes from input file First Volume Added = 0.10 mL 10.00 mL Final Volume Added = $pmH = -log\{m(H+)\}$ 5.9141 = pH = -log[a(H+)]= 5.3205 pmH = -log[m(H+)]6.2386 pH = -log[a(H+)]5.6451 = pmH = -log[m(H+)]pH = -log[a(H+)]6.5870 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+)]pH = -log[a(H+)]10.4406 **=** 9.8493 pmH = -log[m(H+)]10.8825 pH = -log[a(H+)] pmH = -log[m(H+)]10.2955 = 11.2341 pH = -log[a(H+)]10.6594 End of AutoTitration Problem s dir

Directory U1: [SCBABB.FMT.CMS_TESTFILES]

 FMT_FMTC.COM;1
 FMT_HMW_NP_AM.CHEMDAT;1

 NP_NACL_BM.IN;5
 NP_NACL_BM.INGUESS;2

 NP_NACL_BM.OUT;1
 NP_NACL_BM.TITRATE;1

Total of 9 files.

FMT_HMW_NP_AM.RHOMIN;1 NP_NACL_BM.MOLES;1 NP_NACL_BM_JAN08_1523.LOG;1



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

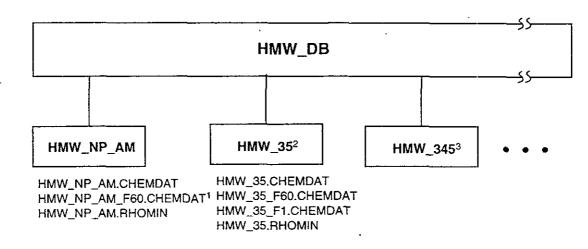
A suggested method for organizing folders or directories while running FMT on the DEC Alpha, Macintosh, or PC platforms is shown in Figures 3 and 4. Using this approach, the user groups

- 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.

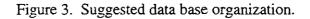
the ouput files in either the same problem-labeled folder or another folder (beneath the problem-labeled folder) labeled with version numbers "V1," "V2," and so on. Both options are shown in Figure 4.

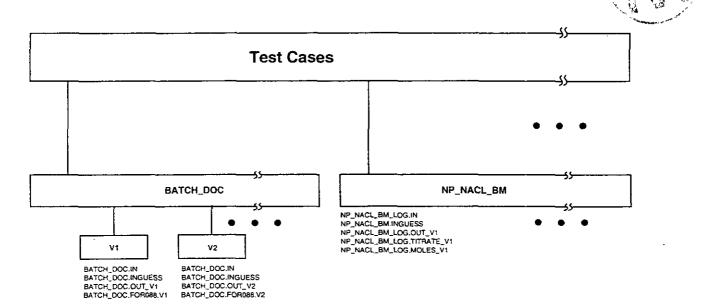


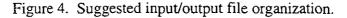
Notes

1. Same as HMW_NP_AM.CHEMDAT, except a declaration of CO2 "solid" fugacity = 60.0 atm was added.

- 2. Contains updates on thermodynamic parameter values and complexation data for Np(V) and Np(V);
- F1 and F60 designate modifications to CHEMDAT file to reflect CO₂ "solid" fugacity at 1 and 60 atm. 3. Folder for future CHEMDAT data bases for Actinides in III, IV, V oxidation states.







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.

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

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

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

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.

Option	Description	Method
LINEAR	add the same constant titrant volume for each iteration increment	$\Delta V_i = DV(2) \times (i-1), i=2,,N_s$, where DV(2) is read from the INPUT file
LOG10	add titrant volumes that increase exponentially from the user specified minimum to maximum volumes	$\frac{\Delta V_i = DV(2) \times e^{(i-2)R}, i=2,,N_s, \text{ with } R=}{\frac{\ln(DV(N_s)) - \ln(DV(2))}{N_s - 2}}, \text{ where } DV(2) \text{ and } DV(N_s) \text{ are read from the INPUT file}}$
ASREAD	add user specified titrant volumes	$\Delta V_i = DV(i)$, i=2,,N _S , where DV(i) values are read from the INPUT file

Table 2.	Titrate Options
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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'

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

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.

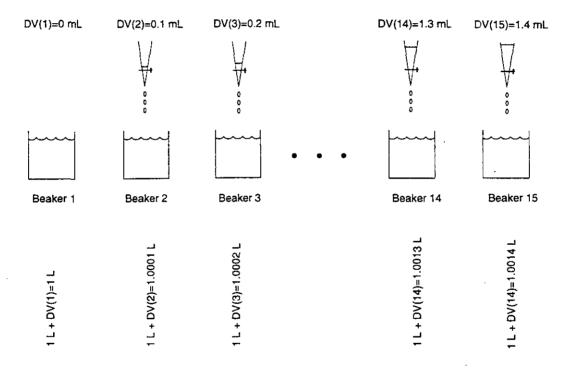


Figure 5. Titration problem using LINEAR option.

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 $i=2, \ldots, NSPACE$.

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])



1.1.

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
	l	1

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 Na₂CO₃•7H₂O(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 NaNpO₂CO₃(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 NaNpO₂CO₃(s) was specified because we are investigating the solubility behavior of this solid as conditions vary, and the large excess allows the amount of solid to change with changing aqueous conditions while keeping the solid phase present.

Examining the TITRATE file, Appendix 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 NaNpO₂CO₃(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 NpO₂⁺, NpO₂OH(aq), NpO₂(OH)₂⁻, NpO₂CO₃⁻, NpO₂(CO₃)₂³⁻, and NpO₂(CO₃)₃⁵⁻,

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).

mCO ₂ ²		<u>_</u>	
	mNp(V) total	mCO_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		

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

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 NpO₂OH(aq) and NpO₂(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

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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.

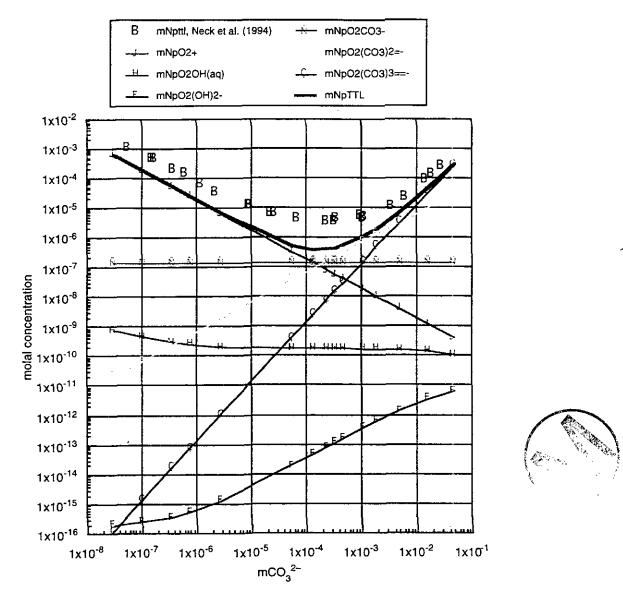


Figure 6. Calculated Total Np(V) and Np(V) Concentrations as a function of CO₃²⁻ concentration in 5.61 molal (5M) NaCl, and comparison with experimental measurements from Neck et al. (1994).

7.0 DESCRIPTION OF INPUT FILES

Of the 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.

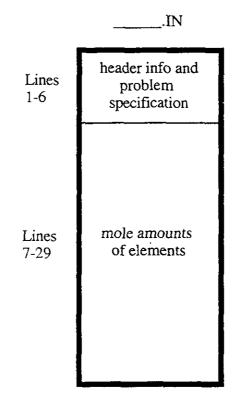


Figure 7. Batch INPUT file.



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).



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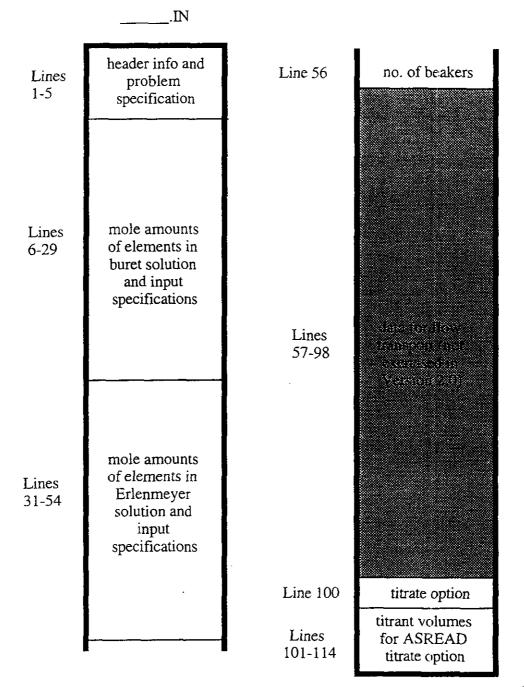


Figure 8. Titrate INPUT file.

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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})

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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:
	CDUMI	'TTTRATE'	'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.

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

Table 6. INGUESS File Parameters for Batch Problem

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.

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



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- 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

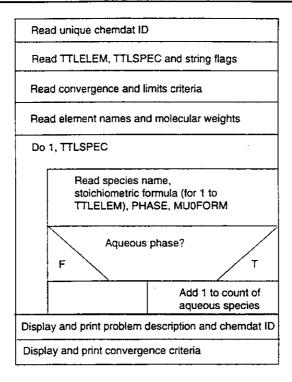
The user should not and is not expected to change the CHEMDAT file. To do so invalidates the QA performed on this data base.

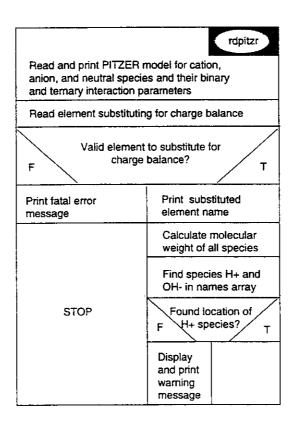
7.3.1 CHEMDAT Data Flow

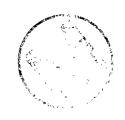
Both the FMT subroutines READDAT and RDPITZR read from the CHEMDAT file. Parameters read from CHEMDAT are echoed or printed to the OUTPUT file. Some parameters are also displayed on the user's screen.

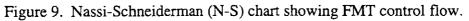
The FMT control flow is illustrated with a Nassi-Schneiderman (N-S) chart (Figure 9). This shows the data flow of the CHEMDAT file in the READDAT subroutine. FMT program variables, TTLELEM and TTLSPEC in the diagram are the total number of elements and the total number of species respectively.

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7.3.2 CHEMDAT Data Sources

The temperature range of the thermodynamic data is specified at 25 $^{\circ}$ C with a few species at 20 $^{\circ}$ C and 30 $^{\circ}$ 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-SO4-OH-HCO3-CO3-CO2-H2O 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, NaClO4, and Na₂CO₃ media are taken from Novak and Roberts (1995). This model for Np(V) chemistry in brines is limited to predominantly NaCl, NaClO4, or Na₂CO₃ 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 Nd³⁺ with a ligand Yⁿ, where n can be positive or negative, and the analogous reaction for Am³⁺:

$$Nd^{3+} + yY^n \leftrightarrow NdY_y^{3+yn}$$
 $\mu_{rxn1}^o = \mu_{NdY_y}^o + yn - \mu_{Nd3+}^o - y\mu_{Yn}^o$ (15)

$$Am^{3+} + yY^{n} \leftrightarrow AmY_{y}^{3+yn}$$
 $\mu_{rxn2}^{o} = \mu_{AmY_{y}}^{o} + yn - \mu_{Am^{3+}}^{o} - y\mu_{Yn}^{o}$ (16)

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

$$\mu_{AmY_y}^{o}^{3+yn} = \mu_{NdY_y}^{o}^{3+yn} + \left[\mu_{Am^{3+}}^{o} - \mu_{Nd^{3+}}^{o}\right]$$
(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 NaHCO3 and Na₂CO₃. media, extending the work for Felmy et al. (1990) to the large carbonate concentrations that could occur in WIPP under disposal scenarios with large CO₂(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 H₃PO₄, $H_2PO_4^{-}$, HPO_4^{2-} , and PO_4^{3-} , as shown in Table 18. The reported standard chemical potentials for

H₃PO₄ and H₂PO₄, 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_{Δ}^{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.

1-1 electrolytes	β ⁽⁰⁾	β ⁽¹⁾	C¢
Na+-ClO ₄	0.0554	0.2755	-0.00118
Na ⁺ -H ₂ PO ₄	-0.0533	0.0396	0.00795
K ⁺ -H ₂ PO ₄	-0.0678	-0.1042	0
H ⁺ -CIO ₄	0.1747	0.2931	0.00819



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2-1 electrolytes	$\frac{4}{3}\beta(0)$	$\frac{4}{3}\beta(1)$	$\frac{2^{5/2}}{3} C^{\phi}$	β ⁽⁰⁾	β ⁽¹⁾	C¢
Na ⁺ -HPO ₄ ²⁻	0.0777	1.954	0.0554	-0.0583	1.466	0.0294
К+-НРО4	0.0330	1.699	0.0309	0.0248	1.274	0.0164
Ca ²⁺ -CIO 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
U02 ⁺ -C1 ⁻	0.5698	2.192	-0.06951	0.4274	1.644	-0.03686
U02 ⁺ -CI0 ₄	0.8151	2.859	0.04089	0.6113	2.144	0.02168

3-1 electrolytes	$\frac{3}{2}\beta^{(0)}$	$\frac{3}{2}\beta^{(1)}$	$\frac{3^{3/2}}{2}C^{\phi}$	β ⁽⁰⁾	β ⁽¹⁾	Сф
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	β ⁽⁰⁾ ,	β ⁽¹⁾	C¢
$UO_2^{2+}-SO_4^{2-}$	0.322	1.827	-0.0176



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

Species	μ <mark>0</mark> /RT	Species	μ _f ^o /RT
NpO ₂ ⁺	-369.127	NaNpO ₂ CO ₃ (s)	-713.707
NpO ₂ OH(am)	-452.642	NpO ₂ CO ₃	-594.492
NpO ₂ OH(aged)	-454.010	NpO ₂ (CO ₃) ₂ ³⁻	-808.403
NpO2OH(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).

$\begin{bmatrix} (0) \\ \beta_{NpO_2^+} - ClO_4^- \end{bmatrix}$	0.312	$\beta_{Na^+-NpO_2CO_3^-}^{(0)}$	0.161	$\beta ((0), Na^{+} NpO_2(CO_3)_3^{5-})$	1.97
$\beta_{NpO_2^+-Cl^-}^{(0)}$	0.169	$\beta ((0), Na^+ - NpO_2(CO_3)_2^{3-})$	0.407	β \s((1),Na ⁺ - NpO ₂ (CO ₃) ₃ ⁵⁻)	16

Table 11.	Dimensionless standard c	chemical potentials for	or Am(III) specie	es from Felmy et al.
		(1990)		·

Species	μ ⁰ / RT
Am ³⁺	-241.694
AmCO ₃ ⁺	-472.06
$\operatorname{Am}(\operatorname{CO}_3)_2^{-}$	-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).

	β ⁽⁰⁾	β(1)	β(2)	C ^{\$}
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 _j ⁰ /RT	Am Species	μ_i^0 / RT
Nd ³⁺	-270.926	Am ³⁺	-241.694
Nd(OH) ⁺ ₂	-422.879	Am(OH) ⁺ ₂	-393.647*
Nd(OH) ⁰ ₃	-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).

	β ⁽⁰⁾	β ⁽¹⁾	β(2)	C¢
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 <mark>0</mark> / 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.

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μ_i^0 / RT	Am Species	μ_{i}^{o} / RT
-270.926	Am ³⁺	241.694
-1425.726	NaAm(CO ₃) ₂ •6H ₂ O(c)	1396.494*
	-270.926	μ_{1}^{2} / K1 -270.926 Am ³⁺

*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).

β ⁽⁰⁾	β ⁽¹⁾	β ⁽²⁾	C ^φ
0	-8.37	0	0
-0.94*	8.1	0	0.418
0	8.37	0	0
-0.94*	8.1	0	0.418
	0 -0.94* 0	0 -8.37 -0.94* 8.1 0 -8.37	0 -8.37 0 -0.94* 8.1 0 0 -8.37 0

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

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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
H3PO4(aq)	-460.90	-460.90	-460.90	-460.90
H ₂ PO ₄	-455.96	-455.960	-455.960	-455.960
нро ₄ ²⁻	-439.404	-439.354	-439.354	-439.367
P04 ³	-410.98	-410.947	-410.947	-410.947
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Table 19. Specific ion interaction parameters for H₃PO₄(aq) from Pitzer and Silvester (1976).

	λ
H ⁺ - H3PO4(aq)	0.290
K ⁺ - H3PO4(aq)	-0.070
$\mathrm{HPO}_{4}^{2-}-\mathrm{H_{3}PO_{4}(aq)}$	-0.400



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

Nd Solid Phase	μ_i^0 / RT	Am Solid Phase	μ_i^o / RT
Nd ³⁺	-270.926		-241.694
<u>.</u>		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

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

	β ⁽⁰⁾	β ⁽¹⁾	β ⁽²⁾	C¢	
$Nd^{3+} - SO_4^{2-}$	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, RFF92, 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.

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)
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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	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	

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	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 ₂ O must always be the first species declared. All aqueous species must be declared before any solid species is declared.
142	DUMMY2, ITEMP	character flag that, when set to 'DG_BYPASS' allows alternate values for the standard chemical potentials to be read from file "bypass" for the first ITEMP species.
143	DUMMY2	character flag that enables the use of the Pitzer activity coefficient model when equal to 'PITZACT'. Any other character string will disable the Pitzer activity coefficient model.
144	NCATION	number of cations for which Pitzer activity coefficient model is used (positive integer) See note below Line 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).

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		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, <math="" and="" anion="" anion-anion="" are="" i="" indices,="" interactions,="" j="" ternary="">\theta_{ij}</j,>	
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, <math="" and="" anion="" anion-anion-cation="" are="" cation="" i="" index,="" indices,="" interactions,="" is="" j="" k="" ternary="" the="">\Psi_{ijk}</j,>	
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	

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		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.
	DUMMY, NSBSTPM, NSBSTRX,	when the flag is 'REDOX'). When this flag is used, it will be follow specifications of NEHRXN (positive integer) redox reactions. This is is unsupported in FMT V2.0. flags and parameters for specifying ion exchange reactions. The val 'IONEX' means that ion exchange reactions are specified on NSBS' permanent substrates and NSBSTRX reactive (soluble) substrates. 'value for DUMMY1 indicates what type of mass-action model to use

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	TTTLE99	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	

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	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 of 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)),	two cation names
	NAMES (ELMAP(1,j))	
	PSI(i,j,k)	cation-cation-anion ternary interaction parameter, Ψ_{ijk}
581-965		table of anion-anion-cation ternary interaction and parameters

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	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.)
1277	(RPLWCHG)	notation that the problem is BATCH (If this were a titration problem)

	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:
		Σ FORMULA(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/m³ 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	~
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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 . . .

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 ...

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



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 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 ...

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 ...

[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 FMT2PO 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 . . .

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 ...



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 ...

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.



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 ...



a.,

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 ...

[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" ...

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 ...

[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



- 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 ...

[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 ...

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 ...

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' ...

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 $\times 1.0 \times 10$ -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' . . .

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 ...

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 . . .

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 . . .

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.

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

Table 26. OUTPUT File Description for Batch (See Appendix M for sample listing.)

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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	TTTLE99, 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

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60-73	l	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 ₂ O, for all species including solids. However, the entry for water is not molality of water, which is invariant, but the mole fraction H ₂ O in the aqueous phase, as noted on line 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

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	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 ₂ O
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	∑CHEMPOT(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 H₂O would have a molal concentration of 1.6×10^{-24} molal, corresponding to a descriptor value of -23.8.) These values are a consequence of the choice of values for the standard chemical potentials of these species. As discussed in the CHEMDAT data base documentation (Section 7.3 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	TTTLË99	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 NS 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.

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1129	r	notation; 10th beaker of Erlenmeyer solution
1129- 1227		ummary information for addition of $DV(10)^*$ to 1 liter of the Erlenmeyer olution
1228	r.	otation; 11th beaker of Erlenmeyer solution
1228- 1326		ummary information for addition of $DV(11)^*$ to 1 liter of the Erlenmeyer olution
1327	r	otation; 12th beaker of Erlenmeyer solution
1327- 1425		ummary information for addition of $DV(12)^*$ to 1 liter of the Erlenmeyer olution
1426	n	otation; 13th beaker of Erlenmeyer solution
1426- 1524		ummary information for addition of $DV(13)^*$ to 1 liter of the Erlenmeyer olution
1525	n	otation; 14th beaker of Erlenmeyer solution
1525- 1623		ummary information for addition of $DV(14)^*$ to 1 liter of the Erlenmeyer olution
1624	n	otation; 15th (last) beaker of Erlenmeyer solution
1624- 1722		ummary information for addition of $DV(15)^{**}$ to 1 liter of the Erlenmeyer olution
1723 TI	NM T	ITRATE filename***
1724 MC	DFNM N	IOLES 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.

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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 ₂ O (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.

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	

Table 29. TITRATE File Description (Appendix R)

1	
AMES(i)	up to 9 columns of species names on a line
SPMOLES(i,j)/ CONST(i)	j th beaker and species molal concentration
IONICST(J)	j th beaker and ionic strength
H(j)	the Eh (an option which is not supported in FMT 2.0)
V(j)*1.d3	titrant volume
IVECT(j)	pH of solution
	CONST(i) CONICST(J) I(j) 7(j)*1.d3

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	N.
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

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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

Appendix A: Sample Screen Display of BATCH_DOC

See Table 1 for explanation of this screen display.

•	Enter chemdat file name to search on: mp_am
7	Enter rhomin file name to search on: np_am
	Enter input file name (without extension): batch_doc
	%(MS-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_HHW_NP_AM_CHEMDAT 'Initial load' FMT_HHW_NP_AM_F60.CHEMDAT 'Initial load'
	Select CHEMDAT name from list above: FMT_HMW_NP_AM.CHEMDAT
с.;-	Your CMS library list consists of:
1	
	%CMS-S-FETCHED, generation 1 of element WP\$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM.CHEMDAT fetched
/ 13 /	Elements in CMS Library WPSNONPA_CMSROOT: [FMT]
20	FMT_HAW_NP_AH.RROWIN 'Initial load' Select RHOMIN name from list above: FMT_HAW_NP_AM.RHOMIN
277	Your CMS library list consists of:
23	
	%CMS-S-FETCHED, generation 1 of element WP\$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM.RHOMIN fetched
28 27	image name: "FMT_FMT2P0"
25 29	
Ŷ.	link date/time: 21-DEC-1995 11:36:28.86
2	
2	
	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
	[.FD.TITRATE]BATCH_DOC.in; to illustrate/document "BATCH" runs FMT V2.0 DATABASE: HHW84/FW86; Np(V)-Na-CO3-OH-C1-C1O4 (NR94);
ģģ.	95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89, FRF90, P91, RFFR92, RFF94, RRFF94)
22	
1.5	Accuracy of reactions is 1.0000E-06
	Minimum elemental abundance is 1.0000E-18
41 42	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50
42 42 43	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50
61 42 43 4	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF, FLAG FITZACT
5 4 2 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF, FLAG PITZACT using PITZER ACTIVITY COEFFICIENT model
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オイロームとオイキシのなちのと、たちちかかできつうたくそうファップではないかったおやいたいがあがかがあるかったのですがあるか。そのうたいできつい、友が	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 FRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.22236400000 Mydrogen 55.1654821000000 Oxygen 0.200000000000000E-002 Potassium 1.000000000000000E-003 Magnesium 1.000000000000000E-004 Calcium 0.1100000000000000E-003 Sulfur 1.000000000000000E-003 Sulfur 1.000000000000000E-003 Sulfur 1.000000000000000E-003 Sulfur 1.000000000000000E-003 Sulfur 1.00000000000000E-003 NegIon 0.00000000000000E-004 Carbon 0.00000000000000E-007 Boron 0.00000000000000E-007 Boron 0.00000000000000E-007 Boron 0.00000000000000E-007 Browine 0.00000000000000E-007 Browine 0.000000000000000E-007 Browine 0.00000000000000E-007 Browine 0.00000000000000E-007 Browine 0.00000000000000E-007 Browine 0.000000000000000E-007 Browine 0.000000000000000E-007 Browine 0.00000000000000000E-007 Browine 0.0000000000000000000000000E-007 Browine 0.000000000000000000E-000 TracerEl 0.00000000000000000000000000000000000
オイルームアオルトロロロガガディロロのためではつけたものです。マンマイはないないである。	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 Coyyen Exiting Subroutine READDAT Char Flags: FLOW/BATCH/ITITRATE BATCH UNUSED this is a BATCH problem Echo of Mole Specifications: nMOLES nEXACT ECHO FRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Mydrogen 55.165482100000 Oxygen 0.20000000000000E-002 Potasium 1.000000000000000E-003 Magnesium 2.000000000000000E-003 Solium 1.00000000000000E-003 Sulfur 1.000000000000000E-004 Calcium 0.1100000000000000E-003 Sulfur 1.00000000000000E-004 Calcium 0.00000000000000E-003 Sulfur 1.00000000000000E-003 Sulfur 1.00000000000000E-000 Psion 0.0000000000000E-000 NgIGn 0.0000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.00000000000000E-000 TricerEl 0.0000000000000E-000 TricerEl 0.000000000000E-000 TricerEl 0.0000000000000E-000 TricerEL
オイドームアオイトの日本でので、日本でもでもつうしたものですがです。これは日本ではないできるのでもしろうかがならないでの中心ですがない。またという	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF, FLAG FITZACT 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 Of Nole Specifications: nMOLES nEXACT EChO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Hydrogen 55.165482100000 Oxygen 0.2000000000000E-002 Potassium 1.00000000000000E-003 Magnesium 1.00000000000000E-003 Solium 1.00000000000000E-004 Calcium 0.10000000000000E-003 Sulfur 1.00000000000000E-003 Sulfur 1.00000000000000E-004 Carbon 0.0000000000000E-004 Carbon 0.0000000000000E-004 Karbon 0.0000000000000E-007 Boron 0.0000000000000E-007 Boron 0.000000000000E-007 Boron 0.000000000000E-000 Ari 0.0000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.00000000000E-000 Magnesi 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 KICI 0.000000000000E-000 KICI 0.000000000000E-000 KICI 0.000000000000E-000 KICI 0.00000000000E-000 Phosphorus 0.00000000000E-000 Ehosphorus 0.00000000000000E-000 Ehosphorus
オイムームイオイキキシの方がたと、この方がどとうなくていたがです。アンドアア	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF, FLAG FITZACT using FITZER 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: nHOLES nEXACT ECHO FRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Bydrogen 55.165482100000 Oxygen 0.2000000000000E-002 Potassium 1.00000000000000E-003 Magnesium 1.00000000000000E-004 Calcium 0.10000000000000E-004 Calcium 0.10000000000000E-004 Calcium 0.10000000000000E-004 Calcium 0.0000000000000E-004 PosIon 0.0000000000000E-004 PosIon 0.00000000000000E-004 PosIon 0.00000000000000E-004 Farban 0.00000000000000E-004 Farban 0.00000000000000E-004 Farban 0.0000000000000E-004 Farban 0.000000000000000E-004 Farban 0.0000000000000E-004 Farban 0.0000000000000E-004 Farban 0.00000000000000E-004 Farban 0.00000000000000E-004 Farban 0.0000000000000E-000 Firban 0.00000000000000E-000 Firban 0.0000000000000E-000 Firban 0.0000000000000E-000 Firban 0.00000000000000E-000 Firban 0.000000000000000000E-000 Firban 0.000000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.0000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.0000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.0000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.0000000000000E-000 Firban 0.000000000000000000000E-000 Firban 0.00000000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.0000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.00000000000000E-000 Firban 0.000000000000000E-000 Firban 0.000000000000000E-
オイムームイオイキキシの方がれているかられてどううかがっていた。アフラインとなられたのであるのでもいろれたので、「ない」のではないないでのないです。ない、ない」ので、	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF, FLAG FITZACT 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 Of Nole Specifications: nMOLES nEXACT EChO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Hydrogen 55.165482100000 Oxygen 0.2000000000000E-002 Potassium 1.00000000000000E-003 Magnesium 1.00000000000000E-003 Solium 1.00000000000000E-004 Calcium 0.10000000000000E-003 Sulfur 1.00000000000000E-003 Sulfur 1.00000000000000E-004 Carbon 0.0000000000000E-004 Carbon 0.0000000000000E-004 Karbon 0.0000000000000E-007 Boron 0.0000000000000E-007 Boron 0.000000000000E-007 Boron 0.000000000000E-000 Ari 0.0000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.00000000000E-000 Magnesi 0.000000000000E-000 Ari 0.000000000000E-000 Ari 0.000000000000E-000 KICI 0.000000000000E-000 KICI 0.000000000000E-000 KICI 0.000000000000E-000 KICI 0.00000000000E-000 Phosphorus 0.00000000000E-000 Ehosphorus 0.00000000000000E-000 Ehosphorus
オペムームイオネルもちちちちち、こちちちむとどううくどうプラップアファイントならないできたいですころんどうであらないないないですかないないですができるの、なからいってもい	<pre>Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT using FITZER ACTIVITY COEFFICIENT model Charge Balance replaces element Cxygen Exiting Subroutine READDAT Char Flags: FLOW/BATCH/TITRATE BATCH UNUSED this is a BATCH problem Echo of Nole Specifications: nHOLES nEXACT ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Mydrogen 55.1654821000000 Cxygen 0.2000000000000000 Sodium 1.000000000000000 Sodium 1.0000000000000000 Sodium 1.000000000000000 Sodium 1.0000000000000000 Sodium 1.00000000000000000 Sodium 1.00000000000000000 Sodium 1.00000000000000000000 Sodium 1.00000000000000000 Sodium 1.0000000000000000000000 Sodium 1.00000000000000000000 Sodium 1.0000000000000000000000 Sodium 1.00000000000000000000 Sodium 1.0000000000000000000000000 Sodium 1.0000000000000000000000000 Sodium 1.000000000000000000000000000000000000</pre>
オペムームとオペルショウガガーと、日本方式でもほうたくもものファインディンティングではないないで、「おいた」ではないではないではない。そうたいでもので、たいに、ないというでもいい。	<pre>Minimum elemental abundance is 1.0000E-18 Sumber of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT using FITZER ACTIVITY COEFFICIENT model Charge Balance replaces element Oxygen Exiting Subroutine READDAT Char Flags: FLOW/BATCH/ITTRATE BATCH UNUSED this is a BATCH problem Echo of Mole Specifications: nMOLES nEXACT ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Hydrogen 55.165482100000 Oxygen 0.200000000000000 Sodium 1.000000000000000 Sodium 1.0000000000000000 Chlorine 1.0000000000000000 Chlorine 1.000000000000000000000 Chlorine 1.000000000000000000000000 Chlorine 1.00000000000000000000000000000 Chlorine 1.000000000000000000000000000000000000</pre>
オクロームでする人もののなちには、このでもできつけていたができっていた。そうに、そうではないからないのではなったのではないないかのないでのないないないないないないです。	<pre>Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT using FITZER ACTIVITY COEFFICIENT model Charge Balance replaces element Cxygen Exiting Subroutine READDAT Char Flags: FLOW/BATCH/TITRATE BATCH UNUSED this is a BATCH problem Echo of Nole Specifications: nHOLES nEXACT ECHO PRINT OF ELEMENT ABUNDANCES IN ONEFLSH 110.222364000000 Mydrogen 55.1654821000000 Cxygen 0.2000000000000000 Sodium 1.000000000000000 Sodium 1.0000000000000000 Sodium 1.000000000000000 Sodium 1.0000000000000000 Sodium 1.00000000000000000 Sodium 1.00000000000000000 Sodium 1.00000000000000000000 Sodium 1.00000000000000000 Sodium 1.0000000000000000000000 Sodium 1.00000000000000000000 Sodium 1.0000000000000000000000 Sodium 1.00000000000000000000 Sodium 1.0000000000000000000000000 Sodium 1.0000000000000000000000000 Sodium 1.000000000000000000000000000000000000</pre>

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Appendix A: Sample Screen Display of BATCH_DOC

Solubility Product Violations S



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Appendix B: Sample Screen Display of Np_NaCl_BM_LOG

Appendix B: Sample Screen Display of Np_NaCl_BM_LOG

See Table 3 for explanation of this screen display.

	Enter chemdat tile 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-LIRSET, library set
1	-CMS-I-SUPERSEDE, library list superseded
-	
:	Elements in CMS Library WP\$NONPA_CMSROOT: [FMT]
. :	
1	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]
	<pre>%CMS-S-FETCHED, generation 1 of element WP\$NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM.CHEMDAT fetched</pre>
	Elements in CMS Library WP\$NONPA_CMSROOT: [FMT]
	FWT_HMW_NP_AM.RHCMIN 'Initial load'
	Select RHOMIN name from list above: FMT_HEW_NP_AM.RHOMIN
	Your CMS library list consists of:
20	WP\$NONPA_CMSROOT: (PMT)
25	ACMS-S-FETCHED, generation 1 of element WP5NONPA_CMSROOT:[FMT]FMT_HMW_NP_AM.RHOMIN fetched
- 11 - 11 - 11	image name: *FMT_FMT2P0*
č.	
30	
21	link date/time: 21-DEC-1995 11:36:28.86
21	linker identification: "All-14"
2	THREE Identification: All-Id
	Entering Subroutine READDAT
	reading chemical species data from CHEMDAT file
	DG_BYPASS flag set to nDG_BYPASS
	Benchmark TITRATE Problem, LOGIO option; Np(V)02 with CO3 in 5.61molal NaCl FMT V2.0
	DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-C1-Clo4 (NR94);
	95.01.31 Am(III)-Na-C1-C33-S04-F04 (FRSR89, FRF90, F91, RFF92, RFF94, RRFF94)
53	
٢.	Minimum elemental abundance is 1.0000E-18
1 . 42	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50
1 . 42 43	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50
122	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT
142020	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT Using FITZER ACTIVITY COEFFICIENT model
142020	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT
人名意思的	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT Using FITZER ACTIVITY COEFFICIENT model
1422455	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT using PITZER ACTIVITY COEFFICIENT model Charge Balance replaces element Oxygen
1.202133.2111111111111111111111111111111	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT using PITZER ACTIVITY COEFFICIENT model Charge Balance replaces element Oxygen Exiting Subroutine READDAT
2 A A A A A A A A A A A A A A A A A A A	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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
<pre>< 4 * * * * * * * * * * * * * * * * * *</pre>	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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
< 4 4 4 4 4 4 4 4 4 5 5 5 5 4 4 4 4 4 4	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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
< 4 4 4 4 4 4 4 4 4 5 5 5 5 4 4 4 4 4 4	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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
イイベルドニイベル こうしちぞく いえひどうしょうざい ううしょう	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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
イイベルバゴイ へんこうひんぞくこう ふたいり ひょうしん	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 Character Flags: I.C. nMOLES nEXACT TEMP is an unused local variable 180000.100000000 TITRATION option requires delta(x)=0.01 meters
イイルム いさく たんきひらりぞく こむしん ないろう しゅうひょう	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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: J.C. nMOLES NEXACT TEMP is an unused local variable 180000.100000000 TITRATION option requires delta(x)=0.01 meters Defining delta(x) as such
イイ れいじょく たいそうひりゃく とびちょうかい ひょうりょう	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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: J.C. nMOLES nEXACT TEMP is an unused local variable 180000.100000000 TITRATION option requires delta(x)=0.01 meters Defining delta(x) as such
とそん ふうさどん んきひらりをくとむちろう しんやんうち いろざつ かけのう たいざつ	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT using PITZER ACTIVITY COEFFICIENT model Charge Balance replaces element Oxygen Exiting Subroutine READDAT Char Flags: FLOM/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
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とんかいふふとん いきひらりをくきひらうそくせつ いんでいうひょうひょうひょうひん くどてもつ たいきん	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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: J.C. nMOLES nEXACT Character Flags: J.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= nDIFFUS CONVEC Parameter UNUSED= nSSDIFF RESTART Parameter Value Read = nRESTART UNUSED Parameter Value Read = nRESTART UNUSED Parameter NULL nULTIDN
とみゃんらぶとんんきおもちぞくとおもちそそせつ ロールやんうちょ ひざつくひろん くどうおんしょうぶん	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 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= nDIFFUS SDIFF Parameter UNUSED= cONVEC SSDIFF Parameter Value Read = RESTART
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イス みつらさ イス しきひらり ぞくとむ ちちそく ぜつ わちく ぞうしん ひろう ひろう ひろう くどび ひらむ しょう キモログ	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 Character Flags: I.C. nMOLES nEXACT TTRATION option requires delta(x)=0.01 meters Defining delta(x) as such DIFFUS Parameter UNUSED= nDIFFUS CONVEC Farameter UNUSED= nDIFFUS CONVEC Farameter UNUSED= nSDIFF RESTART Parameter Value Read = nRESTART UNUSED Parameter FRAC FLO TITRATION Problem: -) Assigning all delta(y) to 0.1 m
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とみんようなとんんこうじちぞくとじじろそそぜつ わちくぎせつ センシア かっこう ひろう くじひゃ くどび ひつこうぶん たむす かっ	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 Character Flags: I.C. nMOLES nEXACT TTRATION option requires delta(x)=0.01 meters Defining delta(x) as such DIFFUS Parameter UNUSED= nDIFFUS CONVEC Farameter UNUSED= nDIFFUS CONVEC Farameter UNUSED= nSDIFF RESTART Parameter Value Read = nRESTART UNUSED Parameter FRAC FLO TITRATION Problem: -) Assigning all delta(y) to 0.1 m
とみ ちゅうさと ちゅうおうりぞく とおろうそそせつ ゆろくぞう サフト	<pre>Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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: J.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= nDIFFUS CONVEC Parameter UNUSED= nDIFFUS CONVEC Parameter Value Read = nRESTART UNUSED parameter FRAC FLO TITRATION problem: -) Assigning all delta(y) to 0.1 m -) Setting % Of nodes in Y-direction to 3 -) Setting NONREACTTVE Porosity to 0.0 </pre>
とみ やいうごとん いこひひり ぞくとひろうそくせつ ゆろく デザウワット おひこうひょうひょう ひざつ くじづみ くぜつ おうこう ふきゅんの アオリ みー	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 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= nDIFFUS CONVEC Parameter UNUSED= nDIFF RESTART Parameter VAlue Read = nEESTART UNUSED Parameter SIDSIFF -) 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 UNUSED HISFDIF LHSFDIF
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とみんしうぶとんんこひひりぞくとひろうそもどうわちくぎがせアメジット おひょうひょうひょう ひろう くじておうひょう ふれしの かうひょう	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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: 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= nDIFFUS CONVEC Parameter UNUSED= nDIFFUS CONVEC Parameter SIDIFFUS CONVEC Parameter SIDIFFUL AMULTINU UNUSED Parameter SIDIFFUL AMULTINU UNUSED parameter FRAC FLO TITRATION Froblem: -) Assigning all delta(y) to 0.1 m -) Setting NONREACTIVE Porosity to 0.0 Char Flags UNUSED UNUSED RHSFDIF LHSFDIF Char Flags UNUSED UNUSED RHSFDIF LHSFDIF Char Flags UNUSED UNUSED RHSFDIF LHSFDIF Char Flags UNUSED UNUSED RHSFDIF LHSFDIF
とみゃいらよとというなられぞくという方をもせつられてぞうかり、シップ、「衣をいうら」のでつうになみてもであられてきたのではであった。ないれたのであった。衣ない	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 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= nDIFFUS CONVEC Parameter UNUSED= CONVEC SSDIFF Parameter UNUSED= CONVEC SSDIFF Parameter Value Read = nESTART 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 UNUSED RHSFDIF LESFDIF Char Flags UNUSED UNUSED NOLES nEXACT TEMP is an unused local variable 9.9999999999999905-021
とみかいうなどというなられぞくという方をも合うわたくぞうかい、シング、などについ、とざいういなかくとどであらた。ないたからないないないないないないないないないない。	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 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= nSDIFF RESTART Parameter UNUSED= nSDIFF RESTART Parameter UNUSED= nSDIFF RESTART Parameter FRAC FLO TITRATION Problem: -) Assigning all delta(y) to 0.1 m -) Setting NONREACTIVE Porosity to 0.0 Char flags UNUSED UNUSED UNUSED ENSFDIF LHSFDIF Char Flags UNUSED UNUSED UNUSED NEACT Char flags UNUSED UNUSED UNUSED NEACT TEMP is an unused local variable 9.9999999999909909090909090909090909090
イス やみらえ イス やさおおちゃくとおおちそ € ぜつらちゃをせっか シックフラント あひゅうちょ ひざつう ひろう くどでおった さきぶんたので ぎらゆ ふたん ゆう	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 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= nSIDIFF RESTART Parameter VAUWEDE CONVEC SSDIFF Parameter VAUWEDE as and a nRESTART UNUSED Parameter VAUWE and a nRESTART UNUSED parameter FRAC FLO TITRATION Problem: -) Assigning all delta(y) to 0.1 m -) Setting NONREACTIVE Porosity to 0.0 Char Flags UNUSED UNUSED INDIES nEXACT TEMP is an unused local variable 9.99999999999999990909999999999090900 Char Flags UNUSED UNUSED INDIES NEXCT TEMP is an unused local variable 9.9999999999999999990900 Char Flags UNUSED UNUSED INDIES NEXCT TEMP is an unused local variable 9.9999999999999090 Character Flags: VPOROS FRELASH VPOROS FRELASH
イス やみらえ イス やさおおちゃくとおおちそ € ぜつらちゃをせっか シックフラント あひゅうちょ ひざつう ひろう くどでおった さきぶんたので ぎらゆ ふたん ゆう	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAG FITZACT 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 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= nSDIFF RESTART Parameter UNUSED= nSDIFF RESTART Parameter UNUSED= nSDIFF RESTART Parameter FRAC FLO TITRATION Problem: -) Assigning all delta(y) to 0.1 m -) Setting NONREACTIVE Porosity to 0.0 Char flags UNUSED UNUSED UNUSED ENSFDIF LHSFDIF Char Flags UNUSED UNUSED UNUSED NEACT Char flags UNUSED UNUSED UNUSED NEACT TEMP is an unused local variable 9.9999999999909909090909090909090909090
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イス ちゅうさく ちゃくひひち ぞくとひろうく € ビウ ねろく ぞち ゼワ・シッシュ フラフラー あかようち いひざう うじろみ とどで おうむ ごうぶ キビロア おうゆ いんたん はってき	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAS FITZACT 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: J.C. nMOLES nEXACT Character Flags: J.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= nDIFFUS CONVEC Parameter UNUSED= cONVEC SDIFF Parameter VAUSED eSIDIFF RESTART Parameter VAUSED aSIDIFF RESTART Parameter VAUSED ALE NUELTINJ UNUSED Parameter SUSHPULL NUELTINJ UNUSED Parameter FLOW TITRATION Problem: -) Assigning all delta(y) to 0.1 m -) Setting # Of nodes in Y-direction to 3 -) Setting # Of nodes in Y-direction to 3 -) Setting NONREACTIVE Porosity to 0.0 Char flags UNUSED UNUSED INSERFIT LINSFOIF Character Flags: VPOROS FRFLASH VPOROS FRFLASH Specifying VARLABLE POROSITY for TITRATION Problem Character Flags: VAR_AO_RHO VAR_AO_RHO FRFLASH
イス みっちょく ちゃくひひり ぞくとひろうく € ぜつ ゆろく そせせび・ション フレシシン マント おひにゅうり いひざつ かひろう とどで おひにょう ふきゆんひ ざう ゆーえん ちゅうたんごひ	Minimum elemental abundance is 1.0000E-18 Number of Aqueous Species is 50 ACTIVITY COEF. FLAS FITZACT 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: J.C. nMOLES nEXACT Character Flags: J.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= nDIFFUS CONVEC Parameter UNUSED= cONVEC SDIFF Parameter VAUSED eSIDIFF RESTART Parameter VAUSED aSIDIFF RESTART Parameter VAUSED ALE NUELTINJ UNUSED Parameter SUSHPULL NUELTINJ UNUSED Parameter FLOW TITRATION Problem: -) Assigning all delta(y) to 0.1 m -) Setting # Of nodes in Y-direction to 3 -) Setting # Of nodes in Y-direction to 3 -) Setting NONREACTIVE Porosity to 0.0 Char flags UNUSED UNUSED INSERFIT LINSFOIF Character Flags: VPOROS FRFLASH VPOROS FRFLASH Specifying VARLABLE POROSITY for TITRATION Problem Character Flags: VAR_AO_RHO VAR_AO_RHO FRFLASH

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Appendix B: Sample Screen Display of Np_NaCl_BM_LOG

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Char Flag is UNUSE Char Flag is UNUSE				DIFF
3.				
A MINERAL DENSITIES,	XG /I	MAR. IN FILE	"RH	CMIN*
e /		,		
$2 \text{ pmH} = -\log[m(H+)]$			z	11.6199
$\delta = pH = -log[a(H+)]$	=	11.7497		11.0135
D pmH = -log[m(H+)]		11./40/	r	5,9141
$f = -\log[a(H+)]$	±	5.3205	_	3,3141
TITRATION Character				
cduml= TITRATE		rg3 rdum2≠ LOG10		
First Volume Added			0 mL	
Final Volume Adde		10.0		
	- 10	10.0	0 1102	
<pre>f pmH = -log[m(H+)]</pre>			=	5,9141
$\Im pH = -log[a(H+)]$	-	5.3205	-	3.3141
: pmH = -log[m(H+)]	-	5.5205	=	6.2386
<pre>pH = -log[a(H+)]</pre>	=	5.6451	-	0.2300
$\frac{1}{2} part = -log[a(H+)]$	-	J.04JI	÷	6.5870
$V_{\rm m} pH = -\log[a(H+)]$	75	5,9936	•	0.5870
(이 pmH = -log(m(H+))	-	3.3330	=	8 6366
'0' pH = -log[a(H+)]	=	7.9427	-	8.5360
() pmH = ~log(m(H+))	_	1.3421	=	N 44455
\bigcirc pH = -log[a(H+)]	÷	8.8722	-	9.4653
pmH = -log[m(H+)]	-	0.0/22	=	9.8154
<pre>>> pH = -log[a(H+)]</pre>	=	9.2225	-	3.6134
(아) pmH = -log[m(H+)]		2.2223	=	10.0620
(; pH = -log[a(H+)]	=	9.4695	-	10.0020
pmH = +log[m(H+)]		5.4055		10,2640
= pH = -log[a(H+)]	=	9.6719	-	10.2040
"' pmH = -log[m(H+)]		5.0.15	æ	10.4406
" pH = -log[a(H+)]	×	9.8493		-0.4400
pmH = -log[m(H+)]		5.0455	=	10,6002
$\Box pH = -log[a(H+)]$		10.0098		20.0002
$\sum pnH = -\log[m(H+)]$			=	10.7468
'l'pH = -log[a(H+)]	=	10.1578		-0.7400
$\Im \operatorname{pmH} = -\log[m(H+)]$			=	10.8825
O pH = -log[a(H+)]	=	10,2955		
<pre>pmH = -log[m(H+)]</pre>			=	11.0086
$(22 \text{ pH} = -\log[a(H+)])$	Ξ	10.4243		
120 pmH = -log(m(H+))			=	11,1257
2~ pH = -log[a(H+)]	=	10.5454		
>>> pmH = -log[m(H+)]			÷	11,2341
<pre>pH = -log[a(H+)]</pre>	=	10.6594		
197 End of AutoTitration	n Pr	oblem		



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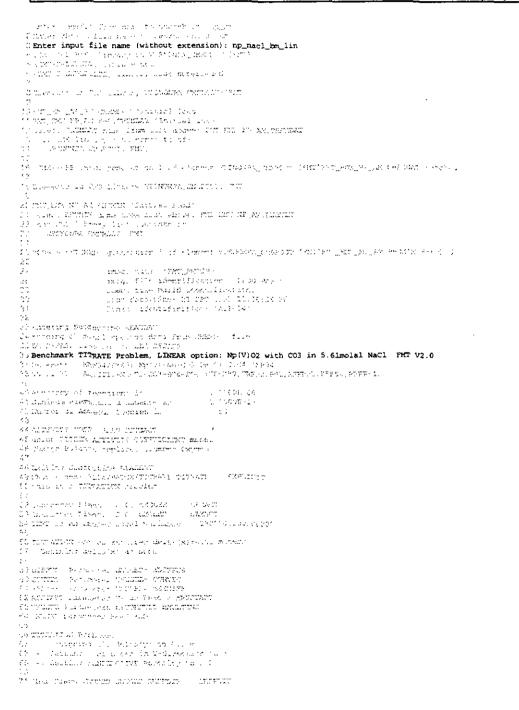
Appendix C Sample Screen Display of Np_NaCl_BM_LIN

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.





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Appendix C Sample Screen Display of Np_NaCl_BM_LIN

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Proto compressione	1456 C 13		: 194	
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a de tras de la contrata	í2 .7	ens ven	27.7	
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er en				
		1 1167		
De ger Der eine Ger eine				
and the second	•	14 A 18 A		
TITRATION Character	r Flags			
cduml= TITRATE		n2= LINEA		
First Volume Add	ed≖		.0 mL	
Final Volume Add	ed =	1.4	0 mL	
25				
$\lim_{n \to \infty} pmH = -\log[m(H_{+})]$			#	5.9141
pH = -log[a(H+)]	=	5.3205		
$\Re pmH = -\log[m(H+)]$			#	6.2386
[X pH = -log[a(H+)]	-	5,6451		
pmH = -log[m(H+)]			=	8.4116
0 pH = -log[a(H+)]	=	7.8183		
'⇔ pmH = -log[m(H+)]	_	0.01/2	×	9,5098
<pre>> pH = -log[a(H+)]</pre>	=	8.9167		
100 pmH = -log[m(H+)]	=		=	9.7906
<pre>100 pH = -log[a(H+)]</pre>	=	9.1977	*	9,9569
°°∕pmH = −log(m(H+))	-	9.3641	a	3.3003
"☆pH = -log[a(H+)] ☆pmH = -log[m(H+)]	-	3.304I	Ŧ	10.0747
<pre>phi = -log(a(H+))</pre>	=	9,4821	-	10.0/4/
':: pmH = -log[m(H+)]	-	2.4021	-	10.1656
$\sum_{n \neq i} pHi = -\log[a(H+)]$	⇒	9,5733		10.2000
$\sum pmH = -\log[m(H+)]$	-	2.2122	-	10.2395
$2pH = -log\{a(H+)\}$	-	9,6473	-	10.2000
* pmH = -log[m(H+)]	=	2.0415	-	10.3015
$\therefore pH = -\log[a(H+)]$	=	9.7095	-	-0.2010
:: pmH = -log[m(N+)]	-	5.7055	£	10.3548
((pH = +log[a(H+)]	-	9,7631	-	10.0010
> pmH = -log[m(H+)]			=	10,4016
22/pH = -log[a(H+)]	=	9.8100	·	
िःः pmH = -log{m(N+)}	-		=	10.4431
10% pH = -log[a(H+)]	-	9.8517		
120 pmH = -log[m(H+)]			*	10,4804
2~ pH = -log[a(H+)]	=	9.8892		
??:pmH = -log[m(H+)]			÷	10.5142
"2 pH = -log[a(H+)]	=	9.9232	~	
	-			

 pH = -log[a(H+)]
 =
 9.9232

 bit
 End of AutoTitration Problem



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Appendix D Sample Screen Display of Np_NaCl_BM

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.





Appendix D Sample Screen Display of Np_NaCl_BM

7. Sant Zinter Although	N		المعتقر م	
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22				
- 77 Novembry test (272,520) - 78	a (124)		<i></i>	- 1964 - M
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— 94 Лидински Стегологуски 199	·		••••	
i en la seraz		يوم محمد ر		
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1992 - 1992 - 1992 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 -	1.53	1 1 24.2	·	f
23				
réalis de la settera				
and the second states of the second				
Columness in the second			•	2
್ಷಕ್ರಿ ಮುಂತಿಡಲ್ಲಾ		2.423		
A TITRATION Character			-	
<pre>cduml= TITRATE reading titrant vo.</pre>				
Preading Citrant Vol Prinst Volume Added		0.14		
> Final Volume Add		10,00		
27				
$65 \text{ pmH} = -\log[m(H+)]$			=	5.9141
야한 pH = -log[a(H+)]	=	5,3205		
10(pmH = -log[m(H+)]			=	6.2386
<pre>PH = -log[a(H+)]</pre>	=	5.6451		-
pmH = -log[m(H+)]			ź	6.5870
10년 pH = ~log[a(H+)]	=	5.9936		6 0000
101 pmH = -log[m(H+)] 102 pH = -log[a(H+)]	=	6.2353	=	6.8286
-10g[m(H+)]	-	0.2000	=	7.2930
[^] pH = -log[a(H+)]	=	6.6996	-	
이야 pmH = -log[m(H+)]			=	8.5359
"\/pH ≠ -log[a(H+)]	*	7.9427		
1 % pmH = -log[m(H+)]			=	8.9250
$\square pH = -\log\{a(H+)\}$	=	8.3317		
$122 \text{ pmH} = -\log[m(H+)]$			=	9.1587
:::pH = -log[a(H+)]	#	B.5655	_	0.0000
$\mathbb{C} \sim pmH = -\log[m(H+)]$	÷	8.7166	=	9.3098
1 ¹⁴ pH * -log[a(H+)] 1 ¹⁵ pmH = -log[m(H+)]	-	0.7100	=	9,4653
<pre>pH = -log[a(H+)]</pre>	=	8.8722	-	
': mmH = -log[m(H+)]			=	9.8154
$\Rightarrow pH = -\log[a(H+)]$	=	9.2225		
".2.2 pamH = +log[m(H+)]			z	10.0620
121 pH = -log[a(H+)]	=	9.4695		
$122 \text{ pmH} = -\log[m(H+)]$			=	10.4406
\$23 pH = -log[a(H+)]	=	9.8493		
<pre>We pmH = -log(m(H+))</pre>	_	10 3055	-	10.8825
(2) pH = -log[a(H+)]	=	10.2955	-	11.2341
"∠^pmH = ~log[m(H+)] *2≤pH = -log[a(H+)]	-	10.6594	-	**.2341
The second secon				

107 End of AutoTitration Problem



Appendix E: Sample Input File "BATCH_DOC.IN"

Appendix E: Sample Input File "BATCH_DOC.IN"

See Table 4 for explanation of this listing.

	'[.FD.TITRATE]BATC: 'CHEMFILE'	H_DOC.in; t	o illustrate/document	"BATCH"	runs'
.*	CHEMPILE				
-	'BATCH', 'UNUSED'				
	'nMOLES', 'nEXACT'				
	1.10222364E+02	, Hydrogen			
	5.51654821E+01				
*	2.00000000E-01	Sodium			
	1.00000000E-02	Potassium			
č.	1.0000000E-02	Magnesium			
· .	1.00000000E-04	Calcium			
	1.10000000E-01	Chlorine			
3		Sulfur			
£ .	1.0000000E-03				
٠,	1.0000000E-04	Carbon			
¢ -	0.0000000E+00	Poslon			
• 5	0.0000000E+00	NegIon			
1.9	0.0000000E+00	Air			
14	1.0000000E-07	Boron			
2 x	0.0000000E+00	Bromine			
24	0.0000000E+00	TracerEl			
2,2	0.0000000E+00	Th(IV)			
20	0.0000000E+00	Am(III)			
11	0.0000000E+00	U(VI)			
21.	0.0000000E+00	Np(V)			
÷.,	0.0000000E+00	C104~(EL)			
	0.0000000E+00	Phosphorus			
24	0.00000C00E+00	Electron			
23	4.90605392E-17	Charge			S. Star James Co.
		-			A.



Appendix F: Sample Input File "Np_NaCl_BM_LOG.IN"

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 NaC1' 'CHEMFILE'

«. 	'TITRATE', 'EXPLIC	CIT',
7 0	'nMOLES', 'nEXACT	,
·-	1.11017363E+02	, Hydrogen
	6.15086815E+01	Oxygen
۰ د	5.61000000E+00	Sodium
12	0.00000000E+00	Potassium
	0.00000000E+00	Magnesium
	0.00000000E+00	Calcium
2	1.61000000E+00	Chlorine
	0.0000000E+00	Sulfur
14	2.00000001E+00	Carbon
13	0.00000000E+00	PosIon
*£ • 5	0.00000000E+00	
	0.00000000E+00	NegIon Air
12	0.00000000E+00	Boron
19		
00	0.0000000E+00	Bromine TracerEl
31	0.00000000E+00 0.00000000E+00	Tracerei Th(IV)
.2.7	0.00000000E+00	
20		Am(III)
26	0.0000000E+00	U(VI)
4.	0.0000000E+00	Np(V)
2.3	0.00000000E+00	ClO4-(EL)
27	0.0000000E+00	Phosphorus
27	0.0000000E+00	Electron
20	-2.22044605E-15	Charge
33		
3; i	'nMOLES', 'nEXACT',	
31	1.11018363E+02	Hydrogen
91 20	1.11018363E+02 1.05508682E+02	Hydrogen Oxyg e n
91 20 24	1.11018363E+02 1.05508682E+02 1.56100000E+01	Hydrogen Oxygen Sodium
91 92 34 34	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00	Hydrogen Oxygen Sodium Potassium
31 22 34 35 35	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Magnesium
31 22 34 35 35 30 37	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Magnesium Calcium
31 20 24 25 25 42 35	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 5.61100000E+00	Hydrogen Oxygen Sodium Potassium Magnesium Calcium Chlorine
31 20 34 35 40 35 35	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 5.61100000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Magnesium Calcium Chlorine Sulfur
81 82 82 83 85 85 85 85 85 85 85 85 85 85 85 85 85	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 5.61100000E+00 0.0000000E+00 1.00000000E+01	Hydrogen Oxygen Sodium Potassium Magnesium Calcium Chlorine Sulfur Carbon
91 28 24 28 20 39 39 39 40 43	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 5.61100000E+00 0.0000000E+00 1.00000000E+01 0.00000000E+01	Hydrogen Oxygen Sodium Potassium Magnesium Calcium Chlorine Sulfur Carbon PosIon
31 22 24 25 25 25 25 25 25 25 25 25 25 25 25 25	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 5.61100000E+00 0.0000000E+00 1.00000000E+01 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Magnesium Calcium Chlorine Sulfur Carbon PosIon NegIon
91 22 24 25 25 25 25 25 25 25 25 25 25 25 25 25	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 5.61100000E+00 0.0000000E+00 1.00000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Magnesium Calcium Chlorine Sulfur Carbon PosIon NegIon Air
91 04 05 05 05 05 05 05 40 40 40 40 40 40 40 40 40 40 40 40 40	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 5.61100000E+00 0.00000000E+00 1.00000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Magnesium Calcium Chlorine Sulfur Carbon PosIon NegIon Air Boron
31 32 4 3 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 5.61100000E+00 0.00000000E+00 1.00000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Magnesium Calcium Chlorine Sulfur Carbon PosIon NegIon Air Boron Bromine
31 32 34 35 35 35 35 4 4 4 4 35 35 4 4 4 35 35 4 4 4 35 35 4 4 4 35 35 4 4 4 35 35 4 35 35 4 4 4 35 35 4 35 35 4 4 35 35 4 35 35 4 35 35 4 35 35 35 35 35 35 35 35 35 35 35 35 35	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 5.61100000E+00 1.00000000E+00 0.0000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Calcium Chlorine Sulfur Carbon PosIon NegIon Air Boron Bromine TracerEl
	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 5.61100000E+00 1.00000000E+00 0.0000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Calcium Chlorine Sulfur Carbon PosIon NegIon Air Boron Bromine TracerEl Th(IV)
31.33.44 (C. 20.35.37.40) 	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.00000000E+00 5.61100000E+00 1.00000000E+00 1.00000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Calcium Chlorine Sulfur Carbon PosIon NegIon Air Boron Bromine TracerEl Th(IV) Am(III)
81 81 42 81 81 81 81 81 81 81 81 81 81 81 81 81	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.0000000E+00 5.61100000E+00 1.00000000E+00 0.0000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Calcium Chlorine Sulfur Carbon PosIon NegIon Air Boron Bromine TracerEl Th(IV) Am(III) U(VI)
31.33.44 (C. 20.35.37.40) 	$1.11018363E+02\\1.05508682E+02\\1.5610000E+01\\0.0000000E+00\\0.0000000E+00\\0.0000000E+00\\5.61100000E+00\\1.00000000E+00\\1.00000000E+00\\0.0000000E+00\\1.0000000E+01$	Hydrogen Oxygen Sodium Potassium Calcium Chlorine Sulfur Carbon PosIon NegIon Air Boron Bromine TracerEl Th(IV) Am(III) U(VI) Np(V)
31.00 4 £ 0 12.30 7 4 4 4 4 4 4 5 4 4 4 4 5 9 5 4 5 4 5 4 5	1.11018363E+02 1.05508682E+02 1.56100000E+01 0.00000000E+00 0.0000000E+00 5.61100000E+00 1.00000000E+00 0.0000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	Hydrogen Oxygen Sodium Potassium Calcium Chlorine Sulfur Carbon PosIon NegIon Air Boron Bromine TracerEl Th(IV) Am(III) U(VI)

FMT, Version 2.0 User's Manual, Version 1.00

Appendix F: Sample Input File "Np_NaCl_BM_LOG.IN" 0.0000000E+00 12 Electron -2.37316632E-15 Charge 51 5£ 15 2.25d3 0.0025d0 1.800001d5 'nDXVARIABLE' :: 'nDIFFUS', 37 CONVEC', at 'nSSDIFF', 'nRESTART', 'nPUSHPULL', 'nMULTINJ', 20 1 20 'nLOTS' 10 . ^ 'nTGRAD' 'LINEAR' 'FRAC FLO' 'nTWO PHASE' 'nMASS TR' З ::-0.1d0 0.2d0 0.3d0 1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF' 35 InmoLES' 'nEXACT' Plain old pure H20 1.11017364E+02 Hydrogen 7,5 5.55086820E+01 Oxygen 0.0000000E+00 Sodium 0.0000000E+00 Potassium 7.5 0.0000000E+00 Magnesium 21 0.0000000E+00 Calcium 22 Chlorine 0.0000000E+00 0.0000000E+00 Sulfur 77 0.0000000E+00 Carbon 0.0000000E+00 PosIon 19 0.0000000E+00 NegIon ь. 0.0000000E+00 23 Air 82 0.0000000E+00 Boron 4.5 0.00000000E+00 Bromine 0.0000000E+00 TracerEl 24 $\delta (\cdot)$ 0.0000000E+00 Pu(III) 0.0000000E+00 Am(III) ÷., 32 0.0000000E+00 U(VI) 0.0000000E+00 33 Np(V)0.0000000E+00 ςč C104-(EL) < (0.0000000E+00 Phosphorus 6.3 0.0000000E+00 Electron 0.0000000E+00 52 Charge ÷.: 34 1.d-12 1.d-20 (fracture, matrix permeabilities) er 'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash) c 'VAR_AQ_RHO' 1074.9d0 anno X DIFF', UNIFORM',0 52 'TITRATE', 'LOG10', 0.1d0, 10.d0, 'nINJSOLIDS'

Appendix G: Sample Input File "NP_NaCl_BM_LIN.IN"

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.

	Benchmark	TITRATE	Problem.	LINEAR	option;	Np(V)02	with	CO3	in	5.61molal	NaCl'
З.	والمتعورية والعدمة والا		* *** }								
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č	5. XX/XXX XX XX 1	1	۱.								
¢	NEXOLES',										
?	1.11.17.1		Hymroger Aller	-							
\$	0.150505		orget.								
4	8.810000		Societ								
::	1.000000		Potassin								
• •	0.000000		Magnesi								
12	0.000000		Calcium								
13	بالمكرية أوالي مراي		Chippin								
12	1.000000		53. <u>É</u> 197								
1.7	3.000000		derbon								
18	0.000000		Pector								
- F	0.000000		Neglor								
6	0.00000										
19	c.000000		Boron								
10	0100000		Eromine								
31	0.000000		<u> TracerE</u>	• ••							
22	0.000000		Th(IV)								
23	0.00000		All (LIII)								
÷ 4	6.000000		U(VE)								1. N.
1.5	0.000000		M(2,7)							÷.,	in the second
D÷			- 0104- (EB							:	
17	0.000000		Phospho							1 1 A.	
Żс	0.000000		Electro								
20	-2.220446	05E-15	Charge							<u> </u>	E /
30										N. Commence	
21	'tMOLES','	NEXACT (
22	1.110183		Eyaroge	~ ~							
23	1.055080	S2E+02	Oxygen								
34	1.561000	的心理中心正	Sedium								
25	0.000000	008+00	Potassi								
30	0.000000	00#400	Magnesi	LIN:							
37	6.656630	00+E00	Calcium								
38	5,611000		Chilorian-								
3	0.000000	.00E-00	Salfar								
40			Carbon								
λ :	0.000000	00 <u>5</u> -00	Peslet								
42	0.000000	100 % - 00	Neçilon								
	6.00000		Adv								
4.4	6.000000	00-200	జంజంగ								

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Appendix G: Sample Input File "NP NaCl BM LIN.IN"
             0.000000002-00
                                                        Brouine
 ÷.
            0.00000002+00
                                                        Cale States EL
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            0.00000002+00
                                                        1.
             0.0000000E+00
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            0.00000002400
                                                        40
             1.00000008<del>.</del>01
                                                        ato na
 2.0
             olippopopoziene
                                                       C_O4-(E1)
             i passeses es
                                                        Nespecto
 12
            C.CCCCCCCCCE+CC
 13
                                                      Sleaterat
         -3.273120308-18 Charpe
 :: ÷
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       -15 012603 0.002500 1.SOCOCLAS (norvariable)
 28
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       "FRAC FIC! "HTWO FRASE "HIMASS IF"
61
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        -01140-01180-01340
       -1.8-7 0.80 0.1529185 0.200 0.80 FREEDIST TERSEDIST
e^{2}e^{2}
      NEXOTES (NEXACT) Plain old pure E20
             0.110175548+02 SycLogen
 71
            5.550262002+01
                                                        Oxygen
71
             ()00000000000000000
                                                     - Codinax
            0.00000005+00
23
                                                       lotassium
            Nacrosizi
 22
 ~:
            Calcium
            0.00000022+00
                                                       ohloríne
7
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                                                        Sel Ser
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                                                        Carbon
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            G.CCCC00000E+60
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            00+E900009300.0
                                                        Branine
33
            C.CCCCCCCC2#00
                                                        TracerEl
24
            00+E0000000E+00
                                                        Fa(III)
55
           0.000000000000
                                                        AT (TII)
28
           0.000000000000
                                                        C(VI)
e7
           0.000000008+00
                                                       N 0 ( V )
23
            0.0000000<u>8</u>+00
                                                    C104-(E1)
\mathcal{A}
            01000000002+00
20
                                                       -Etosphoras
            0.00000002466
                                                        Electros
01
           0.00000000000000 - Charge
3.2
93
          1.d-12 1.d-20 (fracture, matrix permeabilities)
41
M. 'VPOROS' 'FRFLASH' (NOFLASH of FRFLASH, default is all flach)
36 1VAR_AQ_ERO1 1074.540
at (the X DIFF).
ar / UNIFORM / . C
10.00
```

'TITRATE', 'LINEAR', .1, 10, 'NINJSOLIDS'

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Appendix H: Sample Input File "Np_NaCl_BM.IN"

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)02	with	CO3 i	in 5.61molal	NaCl'
2										
ŝ										
	CITERATE',	CERPERCY								
Ē			,							
ċ	'mores',	15EX40	\$							
7			Eveloper							
'n	0.02056		langgeri.	*						
	5.02000		Societ							
5(0.00000		Porassin	117.						
			Nacresi							
:	0.00000		Calcium							
	1.01000		Callouria.							
1	0100000		Salaar							
14	2.00000		daxbon.							
-1	0.00000		Feelon							
.;	1,00000		Kec Ion							
13	0.00000		Aár							
10	6,00000		Boron							
~	0,00000		Frante							
2	1.00000		CocersE:						•	
22	0.00000		TE(TV)							
23	0.00000		$A_{C}(\overline{z}\overline{z}\overline{z})$							
24	0.00000		C (772)							
20	0,00000	004400	Np (M)							
25	0.00000	00+E000	- 0104-FEX	.)						
27	0.00000	000E-00	Phosphor	co2					The second s	
à:	0.00000	0つり至一つり	Electro						A Garage	
20	-2.22044	605 <u>8-1</u> 5	Charles							
30										т. И
31	'tagees',		,							1
3.3	1,11018.		Ry iz oger							
2.5	1.05508		<i>⊡zy g</i> en							
27	1.55130		Sodiun							
9£	0.00000		Polassin							
3	0.00000		Magnesi	17.						
07	6.00000		Calcaum							
5.2	5.01100		and an	<i></i>						
33	5.00000	コンレヨーワウト	Robitar							
ч. (·	1.03000		Carbon 5 -							
16 E	9,00000		Posler							
<i>C</i> ;	0.00000		λζε <u>ις</u> 1 αρτ • •							
13	0.00000		Ad 1							
	5.00000	しいいたかじじ								

管:

z,

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Appendix H: Sample Input File "Np_NaCl_BM.IN"
    Brenime
{\bf e}_{i} \in
    Traces El
41,
    _____
2.5
                   Arr (122)
    C.CCCCCCCCE+CC
1...
    DEVID)
49
                    352 (2)
    1.0000000E+01
20
    C. 0000002400
                    Phospherica
72
    clittleccccccm+CC
                   Flactro:
::
   -5.272122202-15 Obarge
33
55
   15 2.2533 0.002560 1.80000065 - nDNVARIABLE
:
   menterian.
1.0
  COBL/ZOI
$ 2
. TRECIMEN
  -01
88 20 1 20 Malorga 10
C TITORED' LITERS!
A TRANC REON (MINO PEASE) (MEASS TR)
30
   0.145 0.040 0.340
42
   ->.d-7 0.40 0.1829130 0.2d0 0.40 (RASFLEF) (LESFLE)
\mathbb{C}^{2}
   'mnoles' 'rexact' Plair old pure H20
£0
    1.110173642402
                   Eycz coon
1
                   onygen.
    5.55026210B-01
                   Schium
    locassium
   23
   - 6.60000000E+00 - Magreeior
٠.,
   0.0000000E+00 Calcium
12
    0.000000CE+00 Chlerine
20
    c.ccccccccex+00 Sulfur
    0.0000000E+00 Carbon
25
    6.600000E+00
                   1082.02
20
                   Neglon
    0.00000000±00
20
    2、10000000000000000000000000
                    A i z
~ ÷
    0.000000002+00
                    Berez
12
   0.00000000E-00
                    Bronine
TracerEl
    0.0000000E+00
50
                    Fa(III)
   0.0000000E+00
25
                   り、なりつかりのなる差米の心
28
                   0 (V1)
   0.0000000002-00
e i
   0.000000005-00
                     No (M)
83
                   CL04-(BL)
    0.00000008+00
99
    6.0000002+00
                    Phosphon is
22
    6.0000000E-00
                   Electron
31
    なことのでのなないの差異なな。
                   Charge
32
. :
    1.6-12 1.6-20 (fracture, matrix permeabilities)
6.6
  "TPOFOD' THEFLASH" (MORLASH of FRELASH, defailt is all flash)
· • .
5) 「 7為氏」A2_RE51 2074,940
97 1920 X DIFF.
SA TONTFORMAND
22
'TITRATE', 'ASREAD', 0.1d0, 10.d0, 'nINJSOLIDS'
Ha: 0.10000
```

	Appendix H:	Sample	Input	File '	"Np_N	aCl_E	BM.IN"
122	0.14251						
	0.16						
107	0.18						
°	0.20309						
de.	0.22						
100	0.24						
<i></i>	0.26						
	0.28943						
	0.41246						
	0.58780						
•••	1.1938						

.

1.1938
3.4551

. .

10.000



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

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

I.1 Listing

::`*`*

See Table 23 for explanation of this listing.

3 115 'nNE	T' 'nACTCOEF' '	nECHO' ':	nABC	Ð٠																	
00 1.d-6 1	.d-18 .5 1.d0 1.d0																				
																		_			
NegTon'	'Oxygen' 'Sodium' 'Air' 'Boron' 'B	'Potass tomine'	ium' 'Tra	'N cer	El '	esi T	uun. h(IN	י נע ינע	alc Ai	1.1100 m (11)	n,	Chi	ori U(V	ne' Il	- 19 - N	iul Io('	fur V)	· · · C. · C10	arb 04-	on' 'Posion (EL)'	
	us 'Electron' '										,				-					.—.	
.0079 15.9	94 22.98977 39.0	983 24.3																			
28.84 10	81 79.904 0.0 23	2.0381 2	43.0	23	8.0	29	237	. 04	82	99.4	150	63	0.9	74	0.0) 0	. 0				
H20		WATER	2 1	0	0 0	0	0 0	0	00	0 0	0 0	0	٥٥	0	0 0	0	٥	0	1	-95.6635	HMW84
Na+		Na+'																		-105.651	HMW84
K+		K+ '	0.0	0	1 0	0	0 0	0	0 0	0 (0 0	0	0 0	0	0 0	0 0	0	1	1	-113.957	HMW84
Ca++		Ca++ '																		-223.30	HMW84
Mg++		Mg++																		-183.468	HMW84
MgOH+		MgOH+ H+																		-251.94 0.	HMW84 HMW84
H+		L +	10	0	00		••				, ,	Ů.		U		, ,	Ŭ	1	1	Ų.	111004
C1-		¢1-'																		-52.955	HMW84
\$04=		SO4 = '																		-300.386	HMW84
HSO4-		HSO4-																		-304.942	HMW84
OH-		ОН-' НСОЗ-																		-63.435 -236.751	HMW84 HMW84
HCO3- CO3=		CO3= '																		~212.944	HMW84
																			-		
CO2 (aq)		CO2 (ag) '																		-155.68	HMW84
CaCO3 (aq)		CO3 (aq)																		-443.5	HMW84
MgCO3 (aq)	Mg	(CO3 (ag) '	03	O	01	U	υU	1	0 0	0 (υ	Ų	ųΟ	U	0 (. 0	0	0	1	-403.155	HMW84
B(OH)3(aq)	B (O)H)3(ag)'	33	0	0 0	0	0 0	0 1	0 0	0 :	LO	0	0 0	e	0 0	0	0	o	1	-390.81	FW86
B(OH) 4-		B(OH)4-'																		-465.20	FW86
B303 (OH) 4-)3 (OH) 4- '																	1	-963.77	FW86
B405 (OH) 4≖)5 (OH) 4=																		-1239.10	FW86
CaB(OH)4+		B(OH)4+'																		-692.30	FW86
MgB (OH) 4+ Br-	Ma	rB(OH)4+' Br−'																		-651,89 -999,99	FW86 arbitrary
Br- C104-	perchlorat																			-999.99	arbitrary
					<u> </u>		~ ~					~	~ ^	~	<u> </u>		~	0	,	500	
NaOH(aq)	to.titrate.ba	se.only	10	1	00	0	0 10	0	u u a n	00	, 0) ^	0	00	U D	0 0) U) O	0	0		500. 500.	arbitrary arbitrary
HC104 (am)	to.titrate.ac	id.only	1 0	ō	00	õ	ōŏ	ō i	οõ	0 0		ō.	0 0	õ	0 1	ĹŎ	õ	ō	î		arbitrary
Posion	POSIT	IVE.ION	0 0	0	0 0	0	00	0	10	0 (0 0	0	0 0	0	0 0	0 0	0	1	_	0.	arbitrary
NegIon	NEGAT	IVE.ION	00	0	0 0	0	0 0	0 (01	0 (0 0	0	0 0	0	0 0	> 0	ο.	-1		Ο.	arbitrary
Posion(OH)	aq)to.titra	te.base'	11	0	0 Q	0	0 0	0	10	0 (0 0	0	0 0	0	0 0	0 0	0	0		500.	arbitrary
HNegIon (ag	to.titra	te.acid	10	0	00	0	υρ	0	0 1 0 0	Q (0 0	0	υ 0 0 0	0	00) ()) ()	0	0		500. 0,	arbitrary arbitrary
iracer(ag)	conservative	.tracer	ψ¢		00	v			50	0 (. 0	*	0 0			, 0	v	5	*	ν.	arourary
H3P04 (aq)	нз	PO4 (ag) '																	1	-460.90	RFF92
H2PO4-		H2P04-																		-455.96	RFF92
HPO4=		HPO4=																		-439.367	RFF94
PO4 = ~		PO4 = -	04	0	Q O	U	00	0	00	υı	10	0	00	0	0 0	1	0	- 3	Ť	-410.947	RFF94
Np02+		ND02+ '	0 7	0	0 0	0	0 0	0	0 0	0.1	0 0	0	0 0	0	10	0 0	o	1	1	-369.127	N&R94
NpO20H(aq)	NoC	20H(ag)																		-438.518	N&R94
Np02 (OH) 2-	NpC	02 (OH) 2+ '	24	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
Np02C03-	N	p02C03-																		-594.492	N&R94
Np02 (C03) 2		CO312=-																		-808.403	NER94
Np02 (CO3) 3	r=- NpO2(C	.03)3==-'	03	.1 0	, v	υU	0	د ن	0	υŲ	U	00	U	5	· 1	v	u u	-2	*	-1019.918	N&R94
Am+++		Am+++'																	1	-241.694	FRF90
AmCO3+		AmCO3+ '	03	0	0 0	0	0 0	1	0 0	0 (0 0	0	01	0	0.0	0 0	٥	1		-472.060	FRF90
Am(CO3)2~		(CO3)2-1	0.6	0	0 0	0	0 0	2	0 0	0 (D O	0	01	. 0	0 0	0 0	0	-1		-695.880	FRF90
Am (CO3) 3=-		CO3)3=-																		-915.460	FRF90
Am (OH) 2+		um (OH) 2 + '																		-393.647 -462.950	RFFR92 RFFR92
Am (OH) 3 (aq	Am {C	ការខ្មាងជួ)՝	د د	0	5 0	5		5			- 0	v	~ 1		~ .	. 0	5		-		- 14 + 11 2 2
Th++++		Th++++	0 0	0	0 0	0	0 0	0	0 0	0 1	0 0	0	1 0	0	0 0	0 0	0	4	1	-999.99	arbitrary
U02++	U	VI) 02++ '	0 2	0	0 0	0	0 0	0	0 0	0	0 0	C	0 0	1	0 0	0 0	0	2	1	-999.99	arbitrary
	1)Np020	H(accal)	1 3		0 0	n	0 0	¢	0 0	0	00		0 0	0	1 (<u>م</u> د	D	D	2	~454.010	N&R94
Np020H (age Np020H (amo		H(agec)	1 3	ŏ	0 0	0	0 0	ō	0 0	0	0 0	0	0 0	ŏŏ	1 (0 0	ō	ō		-452.642	NER94
NaNp02C03 (;)NaNpC	2CO3 (s) *	0.5	; 1	0 0	0	0 0	1	0 0	0	0 0	0	0 0	0 (1 (0 0	0	0		-713.707	N&R94
)2(s)_DISABLED_D																			999.99	arbitrary

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

		AmOF	1003 (c) '	140	0 0 0 0 0 1 0	0 0 0 0 0 1 0 0 0 0 0 0 2 -569.980 FRF90	
'Am (OH)3 (s)_		Am (C)H)3(s)'	330		00000100000 0 2 -492.294 FRSR89	
'NaAm (CO3)2.	6H2O(c)			2 12 1	0 0 0 0 0 2 0	0 0 0 0 0 1 0 0 0 0 0 0 2 +1396.494 RRFF94 0 0 0 0 0 1 0 0 0 1 0 0 2 -709.750 RFF94	
'AmPO4 (c)	•	Ал	ъРО4 (с) '	040	0 0 0 0 0 0 0 0	000001000100 2-709.750 RFF94	
'CaS04		Anb	ydrite'	04	0001010	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -533.73 HMW84	
'NaK3 (SO4)2_	_Aphthital	lite/Gla	serite'	0 6	1300020	00000000000000000000000000000000000000	
'CaC12.6H20_		_Antarc	ticite'	12 6	0001200	00000000000002-893.65 HMW84	
•CaCO3		Are	gonite	03	0001001	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -455.17 HMW84	
·K2SO4		Ar	canite'	0 4	0200010	00000000000002-532.39 MW84	
'MgC12.6H20_		Bisc	hofite'	12 6	0010200	000000000000002-853.1 HMW84	
*Na2Mg (SO4) 2	4820	Bl	loedite	8 12	2010020	0000000000000002-1383.6 HMW84	
'Mg (QH) 2		P	gucite.	22	0010000	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -335.4 HMW84	
'Na6CO3(SO4)	2	ອືບ	irkeite'	0 11	6000021	00000000000002-1449.4 HMW84	
'CaCO3		C	alcite	03	0001001	0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -455.6 HM:484 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -698.7 HM:484	
'CaC12_4H20_	CaC12	2_Tetrah	ıydrite'	84	0 0 0 1 2 0 0	000000000000002-698.7 HM/w84	
'Ca4C12(OH)6	.13H20Ca	10xych1c	ride A'	32 19	0004200	000000000000002-2658.45 HM/w84	
'Ca2C12{OH}2	.H20Ca	oxychic	mide B'	4 3	0002200	00000000000000000000000000000000000000	
'KMgC13.6H2O		Carr	allite'	12 6	0110300	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -1020.3 HMM84 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -1157.83 HMM84	
'MgSO4 7H20_		Ep	somite'	14 11	0010010	00000000000000000000000000000000000000	
*CaNa2(CO3)2	.5H20	Gayl	.ussite'	10 11	2001002	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -113(.B) HMW84	
111-20-100412		G]	merite'	0 8	2001020		
'Ca504.2H20_			_Gypsum'	46	0 0 0 1 0 1 0	Image Image <th< td=""><td></td></th<>	
'NaCl			Halite'	0 0	1000100	0000000000000002-154.99 HMW84	
'MgSO4 6H20		Hexal	ydrite'	12 10	0010010	000000000000000000000 HMW84	
'KMgC1S04.3H	20	¥	ainite'	67	0110110	000000000000002-938.2 Ними84	
KHCO3_		Kali	cinite'	13	0100001	0000000000000000000 HMW84	
*MgSO4 . H20		Kie	serite'	25	0010010	000000000000002-579.80 HMW84	
*K2Mg (SO4) 2	4H20	1	eonite'	8 12	0210020	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -1403.97 Howels 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -2751.45 Howels 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -2751.45 Howels	
'Na4Ca (S04) 3	2820	_Labil	e_Salt'	4 14	4001030	00000000000000000000000000000000000000	
'MgC03	·	Mac	mesite'	0 3	0010001	00000000000000000000000000000000000000	
'Mo2C1/OH13	4820	Mattheway	loride	11 7	0020100	0 0 0 0 0 0 0 0 0 0 0 0 2 ~1029.6 HM6w84	
'KHS04		Мотг	allite	1 4	0100010	00000000000000000000000000000000000000	
'Na2504 1083		Mire	bilite'	20 14	2000010	0 0 0 0 0 0 0 0 0 0 0 0 0 0 1471 15 MMM 84	
*KRH6 (SOA) 7			senite	6 28	0800070	D D D D D D D D D D D D D D D D D D D	
'NaHCO3		r11 N=1	colite'	1 7	1000001	0000000000000002-343.33 HMW84	
'Na2001 1000		wan	Natron	20 17	2000001	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -1382.78 HMW84	
-Macos .1082		Nes	horite'	6 6	0010001	0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -4382 /8 /MM44	
INCOME (FOAL)	(11)0 Big	_wesque	Cohoon !	12 14	0010001	00000000000000000000000000000000000000	
Langea2(SO4) 4.2H20	Poly	maiite'	4 T9	0212040		
Ca(OH)2		Port1	andite'	2 2	0001000	00000000000000002-362.12 HMW84 00000000000002-577.37 HMW84	
'K8H4 (CO3) 6.	3H20K-S	equicar	ponate	10 21	0800000	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -2555.4 H2M984	
						0 0 0 0 0 0 0 0 0 0 0 0 0 2 -1006.8 HMW84	
KZNaH(CO3)2	.2H2OPC	JCASSIU	LITONA	5 B	1200002	0 0 0 0 0 0 0 0 0 0 0 0 2 -971.74 HMW84	
'K3H(504)2	sesquipota	issium_S	ulfate'	1 8	0300020	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -950.8 HM5W84	
Najh(504)2	Sesquis	ioaium_S	ullate.	1 5	2000020	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -919.6 HM5/84	
'Na2CO3.7H2O	Na2C03	-Heptab	ydrate'	14 10	2000001	0 0 0 0 0 0 0 0 0 0 0 0 0 0 2 -1,094.95 HIMN84	
·KC1		5	ATATCS.	0 0	0100100	00000000000000000000000000000000000000	
'K2Ca(504)2.	#20	Syn	genite	2 9	0201020	0000000000000002-1164.8 HMW84	
'Mg2CaCl6.12	H20	_Tachyb	ydrite'	24 12	0021600	0 0 0 0 0 0 0 0 0 0 0 0 0 2 -2015.9 HDW84	
'Na2SO4		Ther	ardite'	04	2000010	000000000000002-512.35 HHW84	
'Na2CO3.H2O_		Thermor	latrite'	24	2000001	000000000000002-518.8 HMw84	
'Na3H(CO3)2.	2н20		_Trona '	58	3000002	00000000000002-960.38 HM/#84	
'Na2B407.10H	20		Borax'	20 17	2000000	0 0 0 0 0 0 0 2 -\$12.35 HNW84 0 0 0 0 0 0 0 2 -\$12.35 HNW84 0 0 0 0 0 0 2 -\$18.8 HNW84 0 0 0 0 0 0 2 -\$18.8 HNW84 0 0 0 0 0 0 2 -\$60.38 HNW84 0 0 0 0 0 0 0 2 -\$224.16 FN86	
*KB508.4H20_	K-Pents	borate_	(30_C)·	8 12	0 1 0 0 0 0 0	0 0 5 0 0 0 0 0 0 0 0 0 0 2 -1770.26 FW86	
*K2B407.4H20	K-Tetra	aborate_	(30_C)'	8 11	0200000	00400000000002-1663.47 FW86	
'NaBO2.4H20	Sodi	ium_Meta	borate'	86	1000000	00100000000002-761.42 FW86	
'NaB508.5H20	Sodiv	um_Penta	borate'	10 13	1000000	00500000000002-1854.80 FW86	
'NaBO2.NaCl.	2H20Tee	pleite_	(20_C) '	44	2000100	00100000000002-725.77 Fw86	
'nDG_BYPASS'	0						
·PITZACT					•		
						3+, Th++++, UO2++, NpO2+	
20 #Ani Cl	, SO4 , HSO4 ,	OH, HCO3	,CO3,B(C)H)4,B3	103 (OH) 4 , B405 ()4, Br, Am(CO3)2+, Am(CO3)3=+, C1O4+, NpO2(OH)2+, NpC, NpC2,	NpC3, H2PO4, HPO4
6 #Neu CO							
1 .0765							
1 .0765	.2644	.0	.00127		- C1-	HMW84 (beta0, beta1, beta2, cphi)	
1 .01958	1.113	.0	.00497		- SO4=	HMW84	
1.0454	.398	.0	.0		HSO4-	H2MA/84	
	.253	.0	.0044		- OH-	HMW84	
1 .0864	.0411	_ D	.0		- HCO3 -	HDW84	
	1.389	.0	.0044	Ma+	- CO3=	HM284	
1 .0864	. 089	.0	.0114	Na+	- B(OH)4-	FW86	and the second s
1 .0864 1 .0277		.0	.0		B303 (OH) 4-	Fw86	م معنى
1 .0864 1 .0277 1 .0399	910	.0	.0		B405 (OH) 4=	FW86	
1 .0864 1 .0277 1 .0399 10427			.0		Br-		*
1 .0864 1 .0277 1 .0399 10427 1056	910	.0	.0		Am(CO3)2-	RRFF94	
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0	910 40 .0				- Am (CO3)3=-	RRFF94, FRF90	in the second
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0	910 40 .0 -8.37	.0				P91	· · · · · · · · · · · · · · · · · · ·
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0 1 .0 1 .94	910 40 .0 -8.37 8.1	.0 .0	.418		L CTON-		
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0 1 .0 1 .0 1 .0554	910 40 .0 -8.37 8.1 .2755	.0 .0 .0	.418 00118	8 Na+		NR94	
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0 1 .0 1 .0554 1 .0	910 40 .0 -8.37 8.1 .2755 .0	.0 .0 .0	.418 00118 .0	8 Na+ Na+	NpO2 (OH) 2 -	NR94 NR94	
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0 1 .0 1 .0554 2 .0554 1 .0 1 .161	910 40 .0 -8.37 8.1 .2755 .0 .0	.0 .0 .0 .0	.418 00118 .0 .0	8 Na+ Na+ Na+	NpO2(OH)2- NpO2CO3-	NR94	
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0 194 1 .0554 1 .0 1 .161 1 .407	910 40 .0 -8.37 8.1 .2755 .0 .0 .0	0. 0. 0. 0. 0.	.418 00118 .0 .0 .0	8 Na+ Na+ Na+ Na+	NpO2 (OH) 2 - NpO2CO3 - NpO2 (CO3) 2≈-	NR94 NR94	The owners
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0 1 .0 1 .0554 1 .0 1 .161 1 .407 1 1.97	910 40 .0 -8.37 8.1 .2755 .0 .0 .0 .0	0.0 0.0 0.0 0.0	.418 00118 .0 .0 .0 .0	8 Na+ Na+ Na+ Na+ Na+	 NpO2 (OH) 2 - NpO2CO3 - NpO2 (CO3) 2 ≈ - NpO2 (CO3) 3 ≈ = 	NR94 NR94 NR94	The second
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0 1 .0554 1 .0 1 .161 1 .407 1 1.97 19533	910 40 .0 -8.37 8.1 .2755 .0 .0 .0 16. .0396	.0 .0 .0 .0 .0	.418 00118 .0 .0 .0 .0 .0	8 Na+ Na+ Na+ Na+ 5 Na+	 NpO2 (OH) 2 - NpO2 (CO3) - NpO2 (CO3) 2 ≈ - NpO2 (CO3) 3 ≈ = H2PO4 - 	NR94 NR94 NR94 P91	The second
1 .0864 1 .0277 1 .0399 10427 1056 111 1 .0 1 .0 1 .0 1 .0 1 .0554 1 .0 1 .161 1 .407 1 1.97	910 40 .0 -8.37 8.1 .2755 .0 .0 .0 .0	0.0 0.0 0.0 0.0	.418 00118 .0 .0 .0 .0	8 Na+ Na+ Na+ Na+ 5 Na+ Na+	 NpO2 (OH) 2 - NpO2CO3 - NpO2 (CO3) 2 ≈ - NpO2 (CO3) 3 ≈ = 	NR94 NR94 NR94	The second

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

••		-	-			
1	.04835	.2122	.0	00084	K+ C1-	HMW8
1	.04995	.7793	.0	.0	K+ SO4=	HMW84
1 -	. 0003	.1735	.0	.0	K+ HSO4-	KMW8
	1298	.320	.0	.0041	K+ OH-	HMN84
	.0296	013	.0	008	K+ HC03-	HMMB
	.1488	1.43	.0	0015	K+ CO3=	HMW8
	.035	.14	.0	.0	K+ B(OH)4-	Fw86
1 -		,0	.0	.0	K+ B303 (OH) 4-	FW86
		,õ	.0		K+ 8405 (OH) 4=	FW86
	.022			.0		F 160
	.0	.0	.0	.0	K+ Br-	
	. 0	.0	.0	.0	K+ Am (CO3)2-	
	.0	,0	.0	.0	K+ Am (CO3)3=-	
	.0	.0	.0	.0	K+ C104-	
1	.0	. 0	.0	.0	K+ NpO2 (OH) 2-	
1	. 0	.0	.0	.0	K+ Np02C03-	
1	.0	.0	.0	.0	K+ NpO2{CO3}2≓-	
1	.0	, O	. 0	.0	K+ Np02(C03)3==-	
1 -	.0678	-,1042	.0	.0	K+ H2P04-	P91
1	0248	1.274	.0	.0164	K+ HPO4=	P91
1	.3729	3,972	. 0	08680	K+ PO4=-	P91
	.3159	1,614	.0	00034	Ca++ C1-	HMW84
2.	.20	3,1973	-54.24	. 0	Ca++ \$04=	HMW84
1	.2145	2,53	.0	.0	Ca++ HSO4-	HMW84
1 -	. 1747	-,2303	-5.72	.0	Ca++ OH-	HMW8
	. 4	2,977	.0	.0	Ca++ HCO3-	HMW8
	.0	.0	.0	.0	Ca++ C03=	HMW8
	.0	.0	0	.0	Ca++ B(OH)4-	FW86
	.0	.0	.0	.0	Ca++ 8303 (OH) 4-	FW86
		.0	.0	.0	Ca++ B405 (OH) 4=	Fw86
	.0					- 1100
	.0	.0	.0	.0	Ca++ Br-	
	.0	.0	.0	.0	Ca++ Am(CO3)2-	
	.0	.0	.0	.0	Ca++ Am(CO3)3≠-	
	.4511	1.756	.0	00500	Ca++ C104-	P91
1 .	.0	.0	.0	.0	Ca++ NpO2(OH)2-	
	.0	.0	.0	.0	Ca++ NpO2CO3-	
3	.0	.0	.0	.0	Ca++ Np02(C03)2=+	
	. 0	.0	.0	.0	Ca++ NpO2(CO3)3=*	-
	.0	.0	.0	.0	Ca++ H2P04-	
	.0	.0	. C	.0	Ca++ HPO4=	
	.0	0	c	.0	Ca++ P04=-	
						-
	. 35235	1.6815	. C	.00519	Mg++ Cl-	HMW84
	.2210	3.343	-37.23	.025	Mg++ SO4=	HHW8
1	4746	1.729	. C	.0	Mg++ HSO4-	HMM8
1	.0	.0	. C	.0	Mg++ OH-	HMW8
	.329	.6072	. C	. 0	Mg++ HCO3-	HMM18
	.0	.0	.0	.0	Mg++ CO3=	HMW8
	.0	.0	.0	.0	Mg++ B(OH)4-	FW86
	.0	.0	.0	.0	Mg++ B303 (OH) 4-	FW86
	.0	.0	.0	.0	Mg++ B405(OH)4=	Fw86
	.0	.0	.0	.0	Mg++ Br-	
			.0	.0	Mg++ Am (CO3)2-	
	.0	.0	.0			
	.0	.0		.0	Mg++ Am (CO3)3*-	B07
	4961	2.008	.0	.009578		P91
	.0	.0	.0	.0	Mg++ NpO2 (OH) 2-	
	.0	.0	.0	.0	Mg++ NpO2CO3-	
	. 0	.0	.0	.0	Mg++ NpO2 (CO3) 2=-	
3	. 0	٥.	.0	.0	Mg++ NpO2(CO3)3==	-
	.0	.0	.0	.0	Mg++ H2PO4-	
	.0	.0	.0	.0	Mg++ HPO4=	
	.0	.0	.0	. 0	Mg++ PO4=-	
1 ~.	. 10	1.658	.0	.0	MgOH+ Cl-	HMW8
1		.0	.0	.0	MgOH+ SO4 =	HMM8
	.0	. 0	.0	.0	MgOH+ HSO4-	HMW8
	. 0	.0	.0	.0	MgOH+ OH-	HMM8
	.0	.0	.0	.0	MgOH+ HCO3-	HMWB
	.0	.0	.0	.0	MgOH+ CO3=	HMW8
	.0	.0	.0	.0	MgOH+ B(OH)4-	
		.0	.0	.0	MgOH+ B3O3 (OH) 4-	
	.0	.0	.0		MgOH+ B4O5 (OH) 4=	
	.0			.0		
	.0	.0	.0	.0	MgOH+ Br-	
	.0	.0	.0	.0	MgOH+ Am(CO3)2-	
	.0	-0	.0	.0	MgOH+ Am (CO3)3=-	
	.0	.0	. 0	.0	MgOH+ C104-	
1	.0	.0	.0	.0	MgOH+ NpO2 (OH) 2-	
	. 0	.0	.0	. 0	MgOH+ NpO2CO3-	
	.0	.0	.0	. 0	MgOH+ NpO2(CO3)2=	-
	.0	.0	.0	.0	MgOH+ NpO2 (CO3) 3=	
1	.0	.0	.0	.0	MgOH+ H2PO4-	
	.0	.0	.0	.0	MgOH+ HPO4=	
1		.0	.0	.0	MgOH+ PO4=-	
1 1	.0			.0008	н+ ⊂1-	HMM8-
1 1 1	.0	.2945	.0			
1 1 1	.0 .1775	.2945	.0		H+ SO4=	HWMAN
1 1 1 1	.0 .1775 .0298	.0	.0	.0438	H+ SO4=	
1 1 1 1 1	.0 .1775 .0298 .2065	.0 .5556	.0 .0	.0438 .0	H+ HSO4-	HMW8
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	.0 .1775 .0298 .2065 .0	.0 .5556 .0	.0 .0 .0	.0438 .0 .0	H+ HSO4- H+ OH-	HMW8 HMW8 HMW8
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	.0 .1775 .0298 .2065 .0	.0 .5556	.0 .0	.0438 .0	H+ HSO4-	HMW8



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4.	I	.0	. 0	.0	.0	H+ B(OK)4- FW86
27	1	.0	.0	.0	.0	H+ B303 (OH) 4- FW86
201	1	. 0	.0	.0	.0	H+ B405(OH)4= FW86
302	1	.0	.0	.0	.0	H+ Br-
032	1	.0	.0	.0	. 0	H+ Am (CO3)2-
ç	1	.0	.0	.0	.0	H+ Am (CO3)3=-
240	1	.1747	.2931	.0	.00819	H+ C104- P91
250	1	.0	.0	.0	.0	H+ NpO2(OH)2-
207	1	. 0	.0	.0	.0	H+ Np02C03-
	1	.0	.0	, ā	.0	H+ NpO2(CO3)2≠-
20.	1	.0	.0	. 0	.0	H+ NpO2(CO3)3=≈-
273	1	.0	۵.	. D	.0	H+ H2PO4-
4.7	1	.0	.0	٥.	.0	H+ HP04=
27,	1	.0	٥.	.0	. 0	H+ PO4=-
27.0						
227	1	.16	.0	. 0	.0	MgB(OH)4+ Cl- HEW84
<u>.</u>	1	.0	. 0	.0	. 0	MgB(QH)4+ SO4= HMW84
125	1	.0	. D	.0	.0	MgB(OH)4+ HSO4~ HMW84
- C.	1	.0	.0	. 0	.0	MgB{OH}4+ OH- HMW84
274	1	.0	.0	.0	.0	MgB(OH)4+ HCO3~ HMW84
275	1	- 0	.0	.0	. 0	MgB(OH)4+ CO3= HMW84
230	1	. Q	. 0	. Q	.0	MgB(QH)4+ B(OH)4-
22	1	. Q	- 0	.0	.0	MgB(QH)4+ B3O3(QH)4~
262	1	.0	.0	- 0	. 0	MgB(OH)4+ B4O5(OH)4=
40.7	1	.0	.0	.0	.0	MgB(QH)4+ Br-
	1	.0	.0	. 0	.0	MgB(OH)4+ Am(CO3)2-
204	1	.0	-0	.0	- 0	MgB(OH)4+ Am(CO3)3=-
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Appendix I: Listing of HMW_NP_AM.CHEMDAT and References Cited in Listing

MgB(OH)4+ MM(CO3)3=-MgB(OH)4+ C104-MgB(OH)4+ MpO2(OH)2-MgB(OH)4+ NpO2CO3-

MgB(OH)4+ HPO4=

MgB(OH)4+ PO4=-

CaB(OH)4+ C1-

CaB(OH)4+ OH-

CaB(OH)4+ SO4= CaB(OH)4+ HSO4-

CaB(OH)4+ HCO3-

CaB(OH)4+ CO3*

CaB(OH)4+ B(OH)4-CaB(OH)4+ B3O3(OH)4-

CaB(OH) 4+ B405 (OH) 4=

CaB(OH) 4+ Br-CaB(OH) 4+ Br-CaB(OH) 4+ Am(CO3) 2-CaB(OH) 4+ Am(CO3) 3=-CaB(OH) 4+ ClO4-CaB(OH) 4+ NpO2(OH) 2-

CaB (OH) 4+ Np02C03-CaB(OH)4+ NpO2(CO3)2=-CaB(OH)4+ NpO2(CO3)3==-

CaB (OH) 4+ H2PO4-

CaB(OH)4+ HPO4= CaB(OH)4+ PO4=-

Am+++ C1-

Am+++ 504=

Am+++ OH-

/ Am+++ CO3#

Am+++ Br-

Am+++ HSO4-

Am+++ HC03-

Am+++ B(OH)4-

Am+++ B303 (OH) 4-

Am+++ B405 (OR) 4=

Am+++ Am(CO3)2-

Am+++ Am(CO3)3=-Am+++ ClO4-

Am+++ Np02(OH)2-

Am+++ Np02C03-Am+++ Np02(C03)2=-

Am+++ Np02 (C03) 3==-

Am+++ H2PO4-

Am+++ HP04=

Am+++ PO4=-

AmC03+ C1-

AmCO3+ SO4=

AmCO3+ HSO4-

AmCQ3+ HCO3-

AmCO3+ B(OH)4-

AmCO3+ B3O3(OH)4-AmCO3+ B4O5(OH)4=

AmCO3+ Am (CO3) 2-

AmCO3+ Am(CO3)3=-

AmC03+ C03=

AmCO3+ Br-

AmCO3+ OH-

MgB(OH)4+ NpO2(CO3)2=-MgB(OH)4+ NpO2(CO3)3==-MgB(OH)4+ H2PO4-

HMW84

HMW84

HMW84

HMW84

HMW84

FRSR89

RFF94

FRF90

RFF94



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。如何改变是不可能的是不会的改变的改变,这些的效率的变变,也不可能在这些不可能。""我们就是我们就是不能的。" "我们就是我们不能的是不会的改变,不可能是不能能是不是我们不可能在一些不可能。"我们就是我们就是我们就是这些我的,不是不是我们的人们也不是不是我们的人们。

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

949 1 .0 260 1 .0 257 <i>I</i> .0 252 <i>I</i> .0	.0 .0 .0 .0 . <i>0 .0</i> .0 .0	- 0 - 0 - 0 - 0	AmCO3+ C104- AmCO3+ NpO2(OH)2- AmCO3+ NpO2CO3- AmCO3+ NpO2(CO3)2=-
383 1 .0 154 1 .0 255 1 .0 259 2 .0 257	0. 0. 0. 0. 0. 0. 0. 0.	-0 -0 -0 -0	AmC03+ NpO2(C03)3=- AmC03+ H2P04- AmC03+ HP04= AmC03+ P04=-
000 1 .0 34.0 3 .0 55.1 1 .0 75.1 1 .0 75.1 1 .0 75.1 1 .0	0, 0, 0, 0, 0, 0, 0, 0, 0, 0,	-0 -0 -0 -0	Th++++ Cl- Th++++ SO4= Th++++ HSO4- Th++++ ON- Th++++ HCO3-
303 3 0 304 1 0 505 1 0 468 1 0 2557 1 0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0	Th++++ CO3= Th++++ B(OH)4- Th++++ B(OG)(OH)4- Th++++ B4O5(OH)4= Th++++ Br-
HA 1 10 HA 3 10 HA 1 10	0 0 0 0 0 0 0 0 0 0	.0 .0 .0 .0	Th++++ Am(CO3)2- Th++++ Am(CO3)3=- Th++++ ClO4- Th++++ NpO2(OH)2- Th++++ NpO2(CO3-
977 3 10 774 3 10 274 1 10 376 3 10 314 3 10	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0	Th++++ Np02(C03)2=- Th++++ Np02(C03)3==- Th++++ H2P04- Th++++ H2P04- Th++++ HP04= Th++++ P04=-
376 373 1 .4274 260 2 .322 261 1 .0 232 1 .0	1.644 .0 1.827 .0 .0 .0 .0 .0	03686 0176 .0 .0	UO2++ Cl- P91 UO2++ SO4= P91 UO2++ HSO4- UO2++ OH-
250 1 .0 384 2 .0 285 1 .0 285 1 .0 285 1 .0	0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0	UO2++ HCO3- UO2++ CO3- UO2++ B (OH) 4- UO2++ B3O3 (OH) 4- UO2++ B4O5 (OH) 4=
233 1 .0 283 1 .0 383 3 .0 344 1 .6113 87 1 .0	.0.00 .0.00 2.144.00 .0.00	.0 .0 .0 .02158 .0	U02++ Br- U02++ Am (CO3)2- U02++ Am (CO3)3=- U02++ ClO4- P91 U02++ NpO2 (OH)2-
393 1 .0 307 3 .0 308 3 .0 398 1 .0 398 2 .0 393 3 .0	0.0.0 0.0.0 0.0.0 0.0.0 0.00	-0 -0 -0 -0 -0	U02++ Np02(C03) U02++ Np02(C03)2=- U02++ Np02(C03)3==- U02++ H2P04- U02++ HP04= U02++ P04=-
399 40: 1 40: 1 40: 1 40: 1 40: 1 40:	0. 0. 0. 0. 0. 0. 0. 0.	-0 -0 -0 -0	Np02+ Cl- NR94 Np02+ S04= Np02+ H504- Np02+ OH-
xxx4 1 .0 xx35 1 .0 400 1 .0 407 1 .0 404 1 .0 405 1 .0 405 1 .0	.00 .0.0 .0.0 .0.0 .0.0 .0.0 .0.0 .0.0	.0 .0 .0 .0 .0 .0	NpO2+ HCO3- NpO2+ CO3= NpO2+ B(OH)4- NpO2+ B3O3(OH)4- NpO2+ B4O5(OH)4= NpO2+ Br- NpO2+ Br- NpO2+ Am(CO3)2-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	.0 .0 .0 .0 .0 .0 .0 .0	NpO2+ Am (CO3) 3=- NpO2+ Cl04- NR94 NpO2+ NpO2 (CR) 2- NpO2+ NpO2+ NpO2(CG3) 2=- NpO2+ NpO2+ NpO2 (CC3) 3=- NpO2+ NpO2+ HPO4 NpO2+ NpO2+ HPO4= NpO2+
$\begin{array}{cccccccccccccccccccccccccccccccccccc$.07 0. .036 0 0. .005 0. 0 .092 0. 0. 0 0. 0. 0. 0 0. 0. 0. 0 0. 0. 0. 0 0. 0. 0. 0 0. 0. 0. 0 0. 0. 0. 0 0. 0. 0. 0 0. 0. 0. 0 0. 0. 0. 0	. 0. 0. . 0. 0. . 0. 0. . 0. 0. . 0. 0.	0. 0. Ca: (cations 4 thru 13) 0. Mg: (cations 5 thru 13)
	5050 .030. 5 .01 .020 0. 0. 0.	12 .10 .	12 .074 0. SG4: 0. 0. 0. 0. HSO4:

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(anions 2-20) (anions 3-20) (anions 4-20) FMT, Version 2.0 User's Manual, Version 1.00

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

44.2 (1) 44.2 (1) 44.2 (1) 44.4 (1) 44.4 (1) 44.4 (1) 4.4 (1	0. 04 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	.10 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	0. -,10 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	0 - 087 0 0 0 0 0 0 0 0 0 0 0 0 0	0. 0. 0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0.	0.0.	Q. 0. 0. 0.	0. 0. 0. 0. 0. 0.	0.0 0.		OH: HCO3: CO3: B(OH)6 B303(C) B405(C) B405(C) B405(C) B405(C) D40; Np02(C) Np0	(anior (anior (anior)()()()()()()()()()()()()()()()()()()(As 7-20) As 8-20) As 9-20) As 10-20) As 12-20) As 12-20) As 13-20) As 15-20) As 15-20) As 16-20)
		055 015 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0. 0.	-,003 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0 .0 .0 .0	0.0 0.0 0.0 0.0 0.0 0.0 0.0	0 0 0 0 0 0 0 0 0	0. 0. 0. 0. 0. 0. 0. 0. 0.	0.0 0.0 0.0 0.0 0.0 0.0 0.0	.0 .0 .0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0 0 0 0 0	0 0	D Na-C 0 Na-F	ig : igOH :	
866900000000000000000000000000000000000	025 022 .0 011 .0 .0 .0 .0 .0 .0	.0 048 .0 .197 .0 .0 .0 .0 .0	.0 .0 0265 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0. 0. 0.	00000000000000	0.0 0.0 0.0 0.0 0.0 0.0 0.0	0.0 0.0 0.0 0.0 0.0 0.0	.0 .0 .0 .0 .0 .0 .0	- 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0	0 0	0 K -H	ig : igOH :	
	012 .0 015 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0. 0.	0.0.0 0.00 0.00 0.00 0.00 0.00 0.00 0.	0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0. 0.	0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0	0.0	.0 .0 .0 .0 .0 .0	0.0 0.0 0.0 0.0 0.0 0.0	.0 .0 .0 .0 .0 .0 .0 .0	0.000.000.000.000.000.000.000.000.000.		0 Ca-3 0 Ca-3 0 Ca-3 0 Ca-3 0 Ca-3 0 Ca-3 0 Ca-3 0 Ca-3	AgOH: I: AgB (DH) 4+ CaB (OH) 4+ AmCO3+ Th++++ JO2++ NpO2++	
4400 2433 4940 4000 4000 2499 500 500 500	.028 011 .0 .0 .0 .0 .0 .0	.003 .0 .0 .0 .0 .0	.0 .0 .78 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0.	0 0 0 0 0	0. 0. 0. 0. 0. 0.	0 .0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0.	0 0 0 0 0 0 0 0	-0 -0 -0 -0 -0 -0 -0 -0		0 Hg-1 0 Hg-1 0 Hg-2 0 Mg-3 0 Mg-3 0 Mg-3 0 Mg-3 0 Mg-1 0 Mg-1	HgB (OH) 4+ CaB (OH) 4+ Am+++ Am+C3+ Th++++ UO2++ NpO2++	
28868888888888888888888888888888888888	0 0 0 0 0 0 0	0. 0. 0. 0. 9. 0. 9. 0. 0. 0. 0. 0.	0, (<i>0</i> , (0, (0, (0, (0, (0, (0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0.	0 0 0 0 0 0	000000	.0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0.	.0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 MgO 0 MgO 0 MgO 0 MgO 0 MgO 0 MgO	H-H : H-MgB(OH)4+ H-CaB(OH)4+ H-Am+++ H-AmCO3+ H-Th++++ H-UO2++ H-NPO2++	
1975 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	.0 .0 .0 .0 .0	0. 0. 9. 0. 9. 0. 0. 0. 0. 0. 0. 0.	0. 0 0. 0 0. 0 0. 0	0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0.	.0 .0 .0 .0 .0	0.00.00	.0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0.	.0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 H-C 0 H-A 0 H-A 0 H-A 0 H-T 0 H-T	gB (OH) 4+ aB (OH) 4+ m+++ mCO3+ h++++ O2++ pO2++	
514 801 872 872 873 874 874 874 875	0. 0. 0. 0.	0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.	0. 0 0. 0 0. 0	0. 0. 0. 0. 0.	.0 .0 .0 .0 .0	.0 .0 .0 .0 .0	.0 .0 .0 .0 .0	000000000000000000000000000000000000000	0. 0. 0. 0. 0.	.0 .0 .0 .0	.0 .0 .0 .0	0. 0. 0. 0.	0 0	0 0 MgB 0 0 MgE 0 0 MgB 0 0 MgB 0 0 MgB	(OH) 4-CaB (OH) {OH) 4-Am+++ 3(OH) 4-AmCO3+ 3(OH) 4-Th++++ 4(OH) 4-Th++++ 3(OH) 4-NpO2++ 3(OH) 4-NpO2++	4+
520 527 522	.0 .0 .0	.0	0.0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	0. 0. 0.	0 0 0 0 0 0. 0 0 0 0 0. 0 0 0 0 0.	00 CaB	(OH) 4-Am+++ (OH) 4-AmCO3+ 3(OH) 4-Th++++	

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129 122	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.00000000CaB(OH)4-UO2++ .0000000CaB(OH)4-NpO2++
602 582 534	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	0. 0. 0.	.0 .0 .0	0. 20. 0.	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0	.0 0 0 0 0 0 0 0 Am+++-AmCO3+ .0 0 0 0 0 0 0 0 Am+++-Th+++ .0 0 0 0 0 0 0 0 Am+++-TO2++
€ %) 2->	.0	.0	.0	.0	. 0	. 0	- 0	. 0	.0	. 0	.0	.0	. 0	.0000000 Am+++-NpO2++
57 101 151	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	.0 .0 .0	0. 0. 0.	0. 0. 0.	.0 .0 .0	.0 .0 .0	.0 .0 .0	0. 0. 0.	.0 0 0 0 0 0 0 0 AmCO3+-Th++++ .0 0 0 0 0 0 0 0 AmCO3+-UO2++ .0 0 0 0 0 0 0 0 AmCO3+-NPO2++
	.0 .0	.0 .0	.0 .0	.0	.0 .0	.0 .0	. 0 . 0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	. 0 . 0	.0000000 Th++++-U02++ .0000000 Th++++-Np02++
يند. برمور	, C	.0	. 0	.0	.0	.0	.0	.0	. 0	.0	.0	.0	. 0	.0000000 UO2++-NpO2++
となる。 ないに、それ、こののないので、は、は、ないで、	.0014 006 019 .0085 0073 024 .026 .026 .026 .026 .026 .026 .020 .020	00	0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0 025	004 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0 .0 013 .0 .0 .0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		000000000000000000000000000000000000000	000000000000000000000000000000000000000		0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	Cl-SO4: (Na,K,Ca,Mg, Cl-HSO4: MgOH,H,MgB(OH)3, Cl-OH: CaB(OH)4,Am+++, Cl-HCO3: AmCO3+,Th+++, Cl-CO3: UO2++,NpO2+) Cl-B(OH)4: Cl-B3O3(OH)4: Cl-B4C(OH)4: Cl-B4C(OH)4: Cl-Am(CO3)2: Cl-Am(CO3)3: Cl-ClO4-: Cl-NpO2(CO3)3: Cl-NpO2(CO3)2=-: Cl-NpO2(CO3)3==-: Cl-H2PO4-: Cl-PO4=-:
644 677 300 500 500 500 500 500 500 500 500 500	005	05 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0.0 .0	-	.0 .161 . .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	000000000000000000000000000000000000000	000000000000000000000000000000000000000			000000000000000000000000000000000000000	SO4-HSO4: SO4-OH: SO4-OH: SO4-CO3: SO4-B(OH)4: SO4-B3O3(OH)4: SO4-B4O5(OH)4: SO4-B4O5(OH)4: SO4-Am(CO3)2: SO4-Am(CO3)2: SO4-Am(CO3)2: SO4-NPO2(OH)2-: SO4-NPO2(OH)2-: SO4-NPO2(CO3)2=-: SO4-NPO2(CO3)2=-: SO4-NPO2(CO3)3==-: SO4-HPO4=: SO4-PO4=: SO4-PO4=:
144 (48) (58) (58) (58) (58) (58) (58) (58) (5	000000000000000000000000000000000000000	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0		0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	000000000000000000000000000000000000000	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0		.00.00.00.00.00.00.00.00.00.00.00.00.00		.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.00.00 .00.00 .00.00 .00.00 .00.00 .00	HSO4-OH: HSO4-HCO3-: HSO4-B(OB)4-: HSO4-B(OB)4-: HSO4-B4O5(OH)4: HSO4-B4O5(OH)4: HSO4-BT-: HSO4-Am(CO3)2-: HSO4-Am(CO3)2-: HSO4-NpO2(OB)2-: HSO4-NpO2(OB)2-: HSO4-NpO2(CO3)2-: HSO4-NpO2(CO3)2-: HSO4-NpO2(CO3)3=-: HSO4-NpO2(CO3)3=-: HSO4-HPO4-: HSO4-PO4-:
	.0 017 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0. 0. 0. 0.	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	000000000000000000000000000000000000000	- 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0			000000000000000000000000000000000000000	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	. 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0	.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0	OH-HCO3: OH-CO3: OH-StOH: 4: OH-B303(OH)4: OH-B405(OH)4: OH-B405(OH)4: OH-Am(CO3)2: OH-Am(CO3)3: OH-ClO4-: OH-NpO2(OH)2-: OH-NpO2(CO3)3=-: OH-NpO2(CO3)3=-: OH-NpO2(CO3)3=-: OH-NpO2(CO3)3=-: OH-NPO2-: OH-HPO4-: OH-PO4=-:

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Appendix I:	Listing of HMW_NP_	AM.CHEMDAT and	References Cited in Listing
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	.002 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0	.00.00	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0 0 0 0	- 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0	- 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0 .0 .0 .0 .0 .0 .0 .0 .0 .0	 .0 HCO3-CO3: .0 HCO3-B(OH) 4: .0 HCO3-B3O3 (OH) 4: .0 HCO3-B4O5 (OH) 4: .0 HCO3-Am (CO3) 2: .0 HCO3-Am (CO3) 3: .0 HCO3-Am (CO3) 3: .0 HCO3-NpO2 (OH) 2-: .0 HCO3-NpO2 (CO3) 2=-: .0 HCO3-NpO2 (CO3) 3==-: .0 HCO3-H2O2 (CO3) 3==-:
	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0. 0. 0.	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	.6 HC03-HP04=: .0 HC03-P04=: .0 C03-B405(0H)4-: .0 C03-B405(0H)4: .0 C03-B405(0H)4: .0 C03-B405(0H)4: .0 C03-B405(0H)4: .0 C03-Am(C03)3: .0 C03-Am(C03)3: .0 C03-Am(C03)3: .0 C03-Np02(C03)3: .0 C03-Np02(C03)2=-: .0 C03-Np02(C03)3==-; .0 C03
	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	0. 0.000000000000000000000000000000000	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0. 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	.0 CO3-PO4=-: 0 B(OH) 4-B3O3(OH) 4: 0 B(OH) 4-B3O5(OH) 4: 0 B(OH) 4-Br: 0 B(OH) 4-Am(CO3) 2: 0 B(OH) 4-Am(CO3) 3: 0 B(OH) 4-NpO2(OH) 2-: 0 B(OH) 4-NpO2(OH) 2-: 0 B(OH) 4-NpO2(CO3) 2=-: 0 B(OH) 4-NpO2(CO3) 3==-: 0 B(OH) 4-NpO2(CO3) 3==-: 0 B(OH) 4-NPO4=: 0 B(OH) 4-NPO4=: 0 B(OH) 4-NPO4=: 0 B(OH) 4-PPO4=: 0 B(OH) 4-PPO4=:
	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	000000000000000000000000000000000000000	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0	.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0	.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	0.00.00.00.00.00.00.00.00.00.00.00.00.0	.0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0	.0. .0. .0. .0. .0. .0. .0. .0. .0.	.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0	 B3O3 (OH) 4-B4O5 (OH) 4; B3O3 (OH) 4-Br; B3O3 (OH) 4-Am (CO3) 2; B3O3 (OH) 4-Am (CO3) 3; B3O3 (OH) 4-C104-; B3O3 (OH) 4-NpO2 (OH) 2- B3O3 (OH) 4-NpO2 (CO3) 2=-; B3O3 (OH) 4-NpO2 (CO3) 3==-; B3O3 (OH) 4-NpO2 (CO3) 3==-; B3O3 (OH) 4-NpO4=; B3O3 (OH) 4-P04=;
	.0 .0 .0 .0 .0 .0 .0 .0	-0 -0 -0 -0 -0 -0 -0 -0 -0	.0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0	- 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0	.0 .0 .0 .0 .0 .0 .0 .0	0.0 0.0 0.0 0.0 0.0 0.0	0 0 0 0 0 0 0 0 0	0.0 0.0 0.0 0.0 0.0 0.0	.0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0	.0 B405 (OH) 4=Br : .0 B405 (OH) 4=Am (CO3) 2: .0 B405 (OH) 4=Am (CO3) 3: .0 B405 (OH) 4=Cl04-: .0 B405 (OH) 4=NP02 (OH) 2- .0 B405 (OH) 4=NP02 (O3) 2=-: .0 B405 (OH) 4=Np02 (CO3) 2=-: .0 B405 (OH) 4=Np02 (CO3) 3==-: .0 B405 (OH) 4=Np04-: .0 B405 (OH) 4=P04=: .0 B405 (OH) 4=P04=-:
500 641 693 605 606 647 695 605 705	.0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0	0 0 0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0 .0	0. 0. 0. 0. 0. 0. 0. 0.	0 .0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0 .0 .0	 0 Br-Am (CO3) 2: 0 Br-Am (CO3) 3: 0 Br-ClO4-: 0 Br-NpO2(OH) 2-: 0 Br-NpO2(CO3) 2*-: 0 Br-NpO2(CO3) 2*-: 0 Br-H2PO4-: 0 Br-H2PO4-: 10 Br-HPO4=: 10 Br-PPO4=-:
201 202 203 204 205 207 207 207	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0	.0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 Am(CO3)2-Am(CO3)3: .0 Am(CO3)2-ClO4-: .0 Am(CO3)2-NpO2(OH)2-: .0 Am(CO3)2-NpO2(CO3)+: .0 Am(CO3)2-NpO2(CO3)3=-: .0 Am(CO3)2-NpO2(CO3)3=-: .0 Am(CO3)2-H2PO4-: .0 Am(CO3)2-H2PO4-:



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	Appe	naix	r: L	istin	gorr	IMW		_AM	.CHI	SML)A I	and	Rei	terences L	lited in Listing
· 3	.0	. 0	.0	.0	. 0	.0	.0	.0	. 0	.0	. D	. 0	.0	Am (CO3) 2-	P04=-:
· · ·	.0	.0	.0	.0	.0	.0	.0	.0	. 0	.0	.0	.0		Am (CO3)3-	C) 61
712	.0	.0	.0	.0	.0	.0	.0			.0	.0	.0	.0 .0		NpO2 (OH) 2-
212	. 0	.0	.0	.0	. 0	. 0	.0		.0	. 0	.0	.0	. 0		Np02C03-:
714	. 0	.0	.0	.0	. 0	.0	.0			. 0	. 0	. 0	.0		Np02(C03)2=-:
715	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0		.0 .0	.0 .0	.0 .0	.0 .0	0. 0.		NpO2 (CO3) 3≈=-:
717	.0	.0	.0	.0	.0	.0	.0			.0	.0	.0	.0	Am (CO3)3- Am (CO3)3-	
2.3	.0	. 0	.0	.0	.0	.0	.0			.0	.0	.0	.0	Am (CO3) 3-	
19	_		_	_		_	_				_	_			
5 () 7 (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	C104-Np02 C104-Np02	
222	.0	.0	.õ	.0	.0	.0	.0			.0	.0	.0	.0	C104-Np02	
703	.0	. 0	.0	. 0	.0	. 0	.0	.0	.0	. 0	. 0	.0	.0	C104-Np02	(CO3) 3==-:
224	.0	.0	.0	.0	.0	.0	.0			.0	.0	.0	.0	C104-H2PC	
205 725	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0				.0 .0	.0 .0	.0 .0	.0 .0	C104-HP04 C104-P04=	
727															•
7.5	.0	.0	.0	.0	.0	.0	.0			.0	.0	.0	.0		Np02C03-:
201 220	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0			.0 .0	.0 .0	.0 .0	.0 .0		NpO2(CO3)2=-:
23	.0	.0	.0	.0	.0	.0				.0	.0	.0	.0	Np02 (OH) 2	Np02(C03)3==-: -H2P04-:
702	. 0	. 0	. 0	. 0	.0	.0		.0	.0	.0	.0	. 0	.0	Np02 (OH) 2	
7\3 	.0	.0	.0	.0	.0	.0	.0	.0	.0	. Q	.0	.0	.0	Np02 (OH) 2	~P04=-:
5 a 705	.0	.0	.0	.0	. 0	.0	.0	.0	. 0	. 0	. 0	.0	. 0	Np02C03-N	p02 (c03) 2=-:
736	.0	.0	.0	.0	.0	.0	. 0			.o	.0	.0	.0		pO2 (CO3) 3==-:
737	.0	. 0	.0	.0	.0	.0				.0	.0	.0	. 0	Np02C03-H	
53) 753	.0 .0	.0 .0	.0 .0	.0 .0	_0 _0	.0 .0				.0 .0	.0 .0	.0 .0	.0 .0	Np02C03-H Np02C03-P	
74.3	.0	.0	.0	.0					. 0	.0	.0			Np02C03+F	
7.11	. 0	.0	.0	. 0	.0	.0				. 0	.0	. 0	.0		(CO3)3==-:
7/2	.0	.0	.0	.0	.0	.0	.0			.0	.0	.0	.0	NpC2-H2PO	
249 744	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0				.0 .0	.0 .0	.0 .0	.0 .0	NpC2-HPO4 NpC2-PO4=	
743														11pca (01-	•
14.5	. 0	.0	.0	.0	.0	.0				0	.0	. 0	. 0	Np02 (C03)	
742 742	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0	.0 .0				.0 .0	.0 ,0	.0 .0	.0 .0	Np02 (C03)	
240	.0	.0	. 0		. 0					. 0	.0		. 0	Np02 (C03)	3
74.7	.0	.0	.0	. 0	.0	.0				.0	.0	.0	. 0	H2P04-HP0	
261	.0	.0	.0	. 0	.0	.0	.0	.0	.0	.0	.0	.0	.0	H2PO4-PO4	±-;
2525		-													
			0	. 0	0	.0	. 0	0	. O .	0	. 0	. 0	۵	HP04-P04=	
765 784	.0	.0	.0	. 0	.0	.0	. 0	.0	.0.	0	.0	.0	.0	HP04-P04=	-:
784 295	. 100	.051	. 18	3.18	I3 .0	.0.	0.0	. 0	.0		0.0	o c	:02-C	ations	Hintow 8 4
784 748 748	.100	.051	.18	3.18 0.	3.0 0.0	.0. .0.	0.0 0.0	. 0 . 0	.0 .0	.0.	0_(0_(02-0 aco3	Cations -Cations	EDW8 4 EDW8 4
784 788	. 100	.051 .0 .0	. 18	3.18 0.	I3 .0	.0. .0.	0.0	. 0	.0 .0 .0	.0 .0	0.0	0 C 0 C	02-0 aco3 igco3	ations	Hintow 8 4
784 748 748 748 747 747 758 759	.100 .0 .0 097 .0	.051 .0 .0 14 .0	.18	3.18 0. 0. 0. 0.	0.0 0.0 0.0 0.0 0.0	.0. .0. .0. .0. .0.	0, 0 0, 0 0, 0 0, 0 0, 0	.0 .0 .0 .0	.0 .0 .0 .0	.0), 0), 0), 0 , 0	0 C 0 C 0 M 0 B	02-0 aco3 igco3 igco3 igco3	Cations -Cations -Cations)3-Cations DH-Cations	юми в 4 ними в 4 ними в 4 FWB 6
784 798 798 797 797 799 709	.100 .0 .0 097 .0	.051 .0 .0 14	.18	3.18 0. 0. 0. 0.	3.0 0.0 0.0	.0. .0. .0. .0. .0.	0.0 0.0 0.0	.0 .0 .0	.0 .0 .0 .0	.0). 0). 0). 0	0 C 0 C 0 M 0 B	02-0 aco3 igco3 igco3 igco3	Cations S-Cations S-Cations S-Cations	HMW8 4 HMW8 4 HMW8 4
784 758 758 757 759 700 700 700 700 700	.100 .0 .0 097 .0	.051 .0 .0 14 .0 07	.18	3.18 0. 0. 0. 0. 0. 0. 3.	3.0 0.0 0.0 0.0 0.0 0.0	.0 . .0 . .0 . .0 . .0 . .29 .	0, 0 0, 0 0, 0 0, 0 0, 0	.0 .0 .0 .0	.0 .0 .0 .0	.0	0 0 0 0 0 0 0 0 0 0 0 0	0 C 0 C 0 M 0 B 0 M 0 H	02-0 aco3 igco3 igco3 igco3	Cations S-Cations S-Cations S-Cations DH-Cations L-Cations	юми в 4 ними в 4 ними в 4 FWB 6
788 788 788 788 788 789 789 789 789 789	.100 .0 097 .0 .0 .0	.051 .0 .0 14 .0 07 .097 .0	.18	3.18 0. 0. 0. 0. 0.	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	.0 . .0 . .0 . .0 . .29 . .0 .	0, 0 0, 0 0, 0 0, 0 0, 0 0, 0 0, 0	.0 .0 .0 .0 .0	.0 .0 .0 .0 .0	.0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 C 0 M 0 B 0 M 0 M 0 M 0 M	02-0 aco3 igco3 (OH) b020 3PO4 0 0 0 0	Cations S-Cations S-Cations 3-Cations B-Cations S-Cations 0 0 0 0 0 0 0 0	HAW84 HAW84 HAW84 FW86 PS76 CO2-Anions HAW84 CaCO3-Anions HAW84
788 788 788 788 788 788 788 788 788 788	.100 .0 097 .0 005 .0 005	.051 .0 14 .0 07 .097 .0	.18	3.18 0. 0. 0. 0. 0. 3. 0. 0. 0.	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 .	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0	0 0	0 C 0 M 0 B 0 N 0 N 0 N 0 N 0 0	02-0 ac03 bgC03 b(0H) bp020 C3P04 0 0 0 0 0 0	Cations Cations 3-Cations 0-Cations Cations Cations 0	H1W84 H1W84 H1W84 FW86 PS76 CO2-Anions H1W84 CaCO3-Anions H1W84 MgCO3-Anions H1W84
788 788 788 788 788 789 789 789 789 789	.100 .0 097 .0 .0 .0	.051 .0 14 .0 07 .097 .0	.18	3.18 0 0 0 0 0 0 0 0	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 .	0, 0 0, 0 0, 0 0, 0 0, 0 0, 0 0, 0	.0 .0 .0 .0 .0 .0	.0 .0 .0 .0 .0 .0	.0 . .0 . .0 . .0 . .0 .), 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0	0 C 0 M 0 M 0 M 0 M 0 M 0 M 0 M	02-0 aco3 igco3 (OH) b020 3PO4 0 0 0 0	Cations -Cations -Cations 3-Cations B-Cations Cations Cations 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	H1W84 H1W84 H1W84 FW86 FS76 C02-Anions H1W84 CaC03-Anions H1W84 MgC03-Anions H1W84 B(CH)3-Anions FW86
784 765 766 767 759 700 769 700 760 765 765 765 767	.100 .0 097 .0 .0 .0 .0 .0 .0 .0 .0 .091	.051 .0 14 .0 07 .097 .0 .0	.18	3.18 0 0 0 0 0 0 0 0	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 .	0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	0. 0. 0. 0. 0. 0. 0. 0. 0.	.0 .0 .0 .0 .0 .0 .0 .0	.0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 C 0 C 0 B 0 D 0 D 0 D 0 D 0 D 0 D 0 D 0 D	C2-C (aCO3 (9CO3 (9CO3 (0H) (0C) (3PO4 (3PO4 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Cations -Cations -Cations 3-Cations B-Cations Cations Cations 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	H1W84 H1W84 H1W84 FW86 PS76 CO2-Anions H1W84 CaCO3-Anions H1W84 MgCO3-Anions H1W84
784 765 787 759 700 700 700 700 700 700 700 700 700 70	.100 .0 097 .0 .0 005 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 07 .097 .0 .0 .018 .0	.18 	3.18 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 . .0 . .0 . .0 .	0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0 .0 .0 .0		0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 C 0 B 0 B 0 N 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C	02-0 aco3 igco3 (0H) bo20 3P04 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Cations Cations Cations 3-Cations H-Cations Cations 0 0 0 0 0 0 0 0	H1W84 H1W84 H1W84 FW86 PS76 CO2-Anions H1W84 MgCO3-Anions H1W84 B(OH)3-Anions FW86 NpO2OH-Anions PS76
764 765 767 757 759 700 769 700 760 765 765 765 765	.100 .0 097 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 07 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18 	3.18 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2	3 .0 0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 .	0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	0 0 0 0 0 0 0 0 0	.0 .0 .0 .0 .0 .0 .0 .0 .0		0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 C 0 B 0 B 0 N 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C	CO2-C aCO3 igCO4 igCO3 igCO4 igCO3 igCO4 igC	Cations S-Cations S-Cations 3-Cations 3-Cations 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
784 57 57 59 700 13 700 77 59 700 13 700 77 59 700 13 700 77 50 700 70 70 70 70 70 70 70 70 70 70 70 7	.100 .0 097 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 .0 14 .0 07 .097 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18 	3.18 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.	3 .0 0 .0	.0 . .0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 . .0 . .0 . .0 .	0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	0 0 0 0 0 0 0 0 0			0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	02-0 aco3 igco3 (0H) bo20 3P04 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Cations -Cations 3-Cations 3-Cations H-Cations 0 0 0 0 0 0 0 0	H1W84 H1W84 H1W84 FW86 PS76 CO2-Anions H1W84 MgCO3-Anions H1W84 B(OH)3-Anions FW86 NpO2OH-Anions PS76
787 755 7567 735 759 705 705 705 705 705 705 705 705 705 705	.100 .0 097 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 .0 14 .0 07 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18: 	3 .18 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 .	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 . .0 . .0 . .0 .	0 .0 0 .0						02-0 (ac03) (c03)	Cations -Cations 3-Cations 3-Cations H-Cations Cations 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
767 759 769 759 759 700 701 759 700 701 759 700 701 759 700 701 759 700 701 759 700 701 759 700 701 759 759 759 759 759 759 759	.100 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 07 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18: 	3 .18 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 .	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 . .0 . .0 . .0 .	0 .0 0 .0			.0), 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0		C2-C2 (acO3) (OH)	Cations -Cations 3-Cations 3-Cations 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
787 767 759 759 700 700 700 700 700 700 700 700 700 70	.100 .0 097 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 07 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18: 00: 00: 0: 0: 0: 0: 0: -	3 .18 0 - 0 0 - 0 0 - 0 0 - 0 0 - 0 0 - 0 0 - 0 .0 .0 .0 .0 .0 .0 .0	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 . .0 . .0 . .0 .	0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		.0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		C2-C2 (aCO3) (gCO3) (gCO3) (GCH) (gCO3) (GCH) (GCH) (GCH) (GCH) (GCH) (GCH) (GCH) (GCH) (GCH) (GCH) (GCH) (GCH) (GCO3) (GCO	Cations -Cations -Cations 3-Cations -Cations 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
784 787 787 787 787 787 787 787 787 788 788 788 788 788 772 772	.100 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 07 .097 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18: 00: 0	3 .18 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 -	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 . .0 . .0 . .0 . .0 . .0 . .0 . .0 .	00.00 00.000000	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	.0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 C C M 0 M M 0 B M 0 C M 0 C M 0 C M 0 C 0 0 C M 0 C M 0	CO2-CC ACCO3 A	Cations -Cations 3-Cations 3-Cations -Cations 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
784 757 757 757 757 757 757 757 757 757 75	.100 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18 	3 .18 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 -	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 . .0 . .0 . .0 .	0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	.0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 C C C M M 0 0 0 0 0 0 0 0 0 0 0 0 0 0	CO2-CC ACCO3 A	Cations -Cations 3-Cations 3-Cations 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
784 785 787 785 780 780 780 780 780 780 780 780 780 775 775 775 775 775	.100 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 07 .0 .097 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18 	3 .18 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 -	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 . .0 . .0 . .0 . .29 . .0 . .0 . .0 . .0 . .0 . .0 . .0 .	0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0		0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 C C C C C C C C C C C C C C C C C C C	CO2-CC ACCO3 SPC04 SPC04 CO CO CO CO CO CO CO CO CO CO	Cations -Cations 3-Cations H-Cations H-Cations Cations 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
784 767 757 758 759 759 759 759 759 759 759 759 759 759	.100 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 07 .0 .097 .0 .00 .0 .0 0 .0 0 .0 0 .0	.18 	3 .18 0 . 0 . 0 . 0 . 0 . 0 . 0 . 0 .	3 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.0 .0	0 .00 0 .00 0 .00 0 .00 0 .00 0 .00 0 .00 0 .00 0 .00 .00	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	.0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 C C C M 0 M M 0 N N N O O O O O O O O O O O O O O O O	CO2-CC ACCO3 A	Cations -Cations 3-Cations 3-Cations 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
784 7577359 700123007201270077572 7002723557777227777777777777777777777777	.100 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 14 .0 07 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18. 	3 .18 0 - 0 - 0 - 0 - 0 - 0 - 0 - 0 -	3 .0 0 .0 0 .0 0 <td>.0 .0</td> <td>0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0</td> <td>0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0</td> <td>0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0</td> <td>.0</td> <td>), 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0</td> <td>CC CC CC</td> <td>CO2-CO ACCO3 SPC03 SPC04 CO2 CO2 CO2 CO2 CO2 CO2 CO2 CO2</td> <td>Cations -Cations 3-Cations 3-Cations 0 0 0 0 0 0 0 0</td> <td>HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion</td>	.0 .0	0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0 0 .0	0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	.0), 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0 , 0	CC	CO2-CO ACCO3 SPC03 SPC04 CO2 CO2 CO2 CO2 CO2 CO2 CO2 CO2	Cations -Cations 3-Cations 3-Cations 0 0 0 0 0 0 0 0	HMW84 HMW84 HMW84 FW86 PS76 CO2-Anions HMW84 CaCO3-Anions HMW84 MgCO3-Anions HMW84 B(OH)3-Anions HWW84 B(OH)3-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion
784 76777359 701207777777777777777777777777777777777	.100 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.051 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0	.18. 	3 .18 0 - 0 0 - 0 0 - 0 0 - 0 0 - 0 0 - 0 - 0	0 0		0 .00 0 .000 0 .0000 0 .0000 0 .0000 0 .0000 0 .0000 0 .0000 0 .00000 0 .00000 0 .00000000	0. 0. 0. 0. 0. 0. 0. 0. 0. 0.	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0		0	CC	C2-C Cacco3 C2-C Cacco3 C2-C Cacco3 C2-C	Cations -Cations 3-Cations 3-Cations 0 0 0 0 0 0 0 0	HHW84 HHW84 HHW84 FW86 PS76 CO2-Anions HHW84 CaCO3-Anions HHW84 B(OH)3-Anions HHW84 B(OH)3-Anions HW86 NpO2OH-Anions FW86 NpO2OH-Anions PS76 CO2-Cation-Anion (Cations down, Anions across)
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FMT, Version 2.0 User's Manual, Version 1.00

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

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Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

See Table 24 for explanation of this listing.

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33	Cation Ining D							
35	Cacion-Anton B	inary Interaction	raidmeters					
30	Cation	Anion	Beta(0)	Beta(1)	Beta(2)	Cphi	Alpha-Va	lues
	Na+	C1-	0.07650	0.26440	0.00000	0.00127		1-1,1-2,1-3
	Na+ Na+	S04= HS04-	0.01958 0.04540	1.11300 0.39800	0.00000	0.00497		1-1,1-2,1-3
	Na+	OH-	0.08640	0.25300	0.00000	0.00440		1-1,1-2,1-3
4 :	Na+	HC03-	0.02770	0.04110	0.0000	0.0000		1-1,1-2,1-3
	Na+ Na+	CO3= B(OH)4-	0.03990	1.38900	0.00000	0.00440		1-1,1-2,1-3
	Na+	B303 (OH) 4-	-0.04270 -0.05600	0.08900 -0.91000	0.00000	0.01140		1-1,1-2,1-3
45		B405 (OH) 4=	-0.11000	-0.40000	0.00000	0.00000		1-1,1-2,1-3
	Na+ Na+	Br-	0.00000	0.00000	0.00000	0.00000		1-1,1-2,1-3
13		Am(CO3)2- Am(CO3)3=-	0.00000	-8.37000 8.10000	0.00000	0.00000		1-1,1-2,1-3
-		C104-	0.05540	0.27550	0.00000	-0.00118		1-1,1-2,1-3
20 01		NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000		1-1,1-2,1-3
	Na+ Na+	Np02C03- Np02(C03)2=-	0.16100 0.40700	0.00000 0.00000	0.00000 0.00000	0.00000		1-1,1-2,1-3
53		NpO2 (CO3) 3==-	1.97000	16.00000	0.00000	0.00000		1-1,1-2,1-3
	Na+	H2P04-	-0.05330	0.03960	0.00000	0.00795		1-1,1-2,1-3
	Na+ Na+	HPO4= PO4=-	-0.05830 0.17810	1.46600	0.00000	0.02940		1-1,1-2,1-3
	K+	Cl-	0.04835	3.85100 0.21220	0.00000 0.00000	-0.05154 -0.00084		1-1,1-2,1-3
55		S04=	0.04995	0.77930	0.00000	0.00000		1-1,1-2,1-3
59 60		HSO4 - OH-	-0.00030	0.17350	0.00000	0.00000		1-1,1-2,1-3
£ :		HC03-	0.12980 0.02 9 60	0.32000 -0.01300	0.00000 0.00000	0.00410		1-1, 1-2, 1-3 1-1, 1-2, 1-3
02		CO3=	0.14880	1.43000	0.00000	-0.00150	(2.0,12)	1-1,1-2,1-3
-03 -64		B (OH) 4-	0.03500	0.14000	0.00000	0.00000		1-1,1-2,1-3
	K+ K+	B3O3 (OH) 4- B4O5 (OH) 4≖	-0.13000 -0.02200	0.00000	0.00000	0.00000		1-1,1-2,1-3
ec.		Br-	0.00000	0.00000	0.00000	0.00000		1-1,1-2,1-3 1-1,1-2,1-3
	K+	Am (CO3) 2-	0.00000	0.00000	0.00000	0.0000		1-1,1-2,1-3
44 03	K+	Am (CO3)3=-	0.00000 0.00000	0.00000	0.00000	0.00000		1-1,1-2,1-3
?>		C104- Np02 (OH) 2-	0.00000	0.00000	0.00000 0.00000	0.00000		1-1,1-2,1-3
73	K+	Np02C03-	0.00000	0.00000	0.00000	0.00000		1-1,1-2,1-3
2	K+	Np02 (C03) 2=-	0.00000	0.00000	0.00000	0.00000	(2.0,12)	1-1,1-2,1-3
: 3 : 4	K+	NpO2 (CO3)3==- H2PO4-	0.00000 -0.06780	0.00000 -0.10420	0.00000	0.00000		1-1,1-2,1-3
25	K+	HPO4=	0.02480	1.27400	0.00000	0.01640		1-1,1-2,1-3 1-1,1-2,1-3
25		P04=-	0.37290	3.97200	0.00000	-0.08680	(2.0,12)	1-1,1-2,1-3
	Ca++ Ca++	C1- SO4=	0.31590 0.20000	1.61400 3.19730	0.00000	-0.00034		1-1,1-2,1-3
	Ca++	HSO4-	0.21450	2.53000	-54.24000 0.00000	0.00000	(1.4, 12) (2.0, 12)	2-2 1-1,1-2,1-3
	Ca++	OH-	-0.17470	-0.23030	-5.72000	0.0000	(2.0,12)	1-1,1-2,1-3
	Ca++ Ca++	NC03-	0.40000	2.97700	0.00000	0.00000		1-1,1-2,1-3
		C03 =	0.00000	0.00000	0.00000	0.00000	(1.4, 12)	2-2



	rippendix 3. C	/01:01:102		··_···		-	
22	Ca++	B (OH) 4 ~	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
54	Ca++	B303 (OH) 4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
45	Ca++	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
25	Ca++	Br-	0.00000	0,00000	0.00000	0.00000	(2.0,12) 1-1,1+2,1-3
÷ 7	Ca++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
5 2 2	Ca++	Am (CO3)3=-	000000.0	00000.0	00000.0	0.00000	(1.4.50) 2-(n>2)
8.4		C104-	0.45110	1.75600	0.00000	-0.00500	(2.0, 12) 1-1, 1-2, 1-3
22	Ca++	Np02 (OH) 2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
	Ca++	Np02C03- Np02(C03)2=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
ż	Ca++ Ca++	Np02(C03)3==-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
	Ca++	H2P04-	0.00000	0,00000	0.00000	0.00000	(2.0.12) 1-1,1-2,1-3
05	Ca++	HPO4=	0.00000	0.00000	0.00000	0.00000	(1.4,12) 2-2
17	Ca++	P04=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
1	Mg++	C1-	0.35235	1.68150	0.00000	0.00519	(2.0.12) 1-1.1-2.1-3
× 2	Mg++	SO4=	0.22100	3.34300	-37.23000	0.02500	(1.4.12) 2-2
2 S - 2	Mg++	H504-	0.47460	1.72900	0.00000	0.00000	(2.0, 12) 1-1,1-2,1-3 (2.0, 12) 1-1,1-2,1-3
• •	Mg++	OH- HCQ3-	0.00000 0.32900	0.00000 0.60720	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
5.0	Mg++ Mg++	CO3=	0.00000	0.00000	0.00000	0.00000	(1.4,12) 2-2
-03	Mg++	B (OH) 4-	0.00000	0.00000	0.00000	0.00000	{2.0,12} 1-1,1-2,1-3
101	Mg++	B3Q3 (OH) 4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
	Mg++	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
16 2 1	Mg++	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
1.17	Mg++	Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
7.7	Mg++	Am (CO3)3=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2- $(n>2)(2.0,12) 1-1 1-2 1-3$
	Mg++	C104- Np02(OH)2-	0.49610 0.00000	2.00800 0.00000	0.00000	0.00958	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
:::	Mg++ Mg++	Np02(0R)2-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) $1-1, 1-2, 1-3(2.0, 12)$ $1-1, 1-2, 1-3$
	Mg++ Mg++	NpO2 (CO3) 2=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2- $(n>2)$
	Mg++	Np02 (C03) 3==-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2- $(n>2)$
۰÷.;	Mg++	H2P04~	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
1 C	Mg++	PQ4=-	0.00000	0.00000	0.00000	0.00000	(1, 4, 50) 2 - (n > 2)
**;	MgOH+	C1-	~0.10000	1.65800	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	MgOH+	S04= HS04-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
12	MgOH+ MgOH+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
•	MgOH+	HCO3-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
4.4.	MgOH+	C03=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
122	NgOH+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
*2÷	MgOH+	B303 (OH) 4-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
- 25	MgOH+	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
1.25	MgOH+	Br-	0.00000	0.00000	0.00000	0.00000	$\{2, 0, 12\}$ 1-1, 1-2, 1-3
	MgOH+	Am (CO3)2- Am (CO3)3≠-	0.00000	0.00000	0.00000	0.00000	{2.0,12} 1-1,1-2,1-3 {2.0,12} 1-1,1-2,1-3
12.5	MgOH+ MgOH+	C104~	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
3.5	MgOH+	Np02 (OH) 2-	0.00000	0.00000	0.00000	0.0000	(2.0,12) 1-1,1-2,1-3
134	MgOH+	Np02C03-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
1 52	MgOH+	Np02(C03)2=~	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
133	MgOH+	Np02 (C03) 3=*-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
134	MgOH+	H2P04- HP04*	0.00000	0.00000 0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
13: 13:	MgOH+	PO4=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
	MgOH+ H+	c1-	0.17750	0.29450	0.00000	0.00080	(2.0,12) 1-1,1-2,1-3
- 5	H+ H+	S04=	0.02980	0.00000	0.00000	0.04380	(2.0,12) 1-1,1-2,1-3
1.5	H+	HS04-	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
171	H+	нсоз-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) $1-1, 1-2, 1-3$
- 4.2	H+	C03=	0.00000	0.00000	0.00000 0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
743 742	H+ K+	B (OH) 4- B303 (OH) 4-	0.00000 0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
145		B405 (OR) 4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
140	H+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0.12) 1-1,1-2,1-3
• • •	H+	Am (CO3)2-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
160	H+	Am (CO3)3=-	0.00000	0.00000	0.00000	0.00000	(2,0,12) 1-1,1-2,1-3
- 3	H+	C104-	0.17470	0.29310	0.00000	0.00819	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
) 171	н+ н+	Np02 (OH) 2-	0.00000	0.00000 0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
162		Np02C03- Np02(C03)2*~	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
155	н.	NpO2 (CO3) 3==-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
+ 6. e.	H-	H2P04-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
5 ÷ 3	H+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	H+	P04=-	0.00000	0.0000	0.00000	0.00000	(2.0, 12) $1-1, 1-2, 1-3$
	MgB (OH) 4+	C1-	0.16000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
168 189		S04=	0.00000	0.00000 0.00000	0,00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
1079 1453	MgB (OH) 4+ MgB (OH) 4+	HSO4- OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
- 6.5	MgB(OH)4+	HC03-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
141	MgB(OH)4+	C03=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
N 15	HgB (OH) 4+	B(OH)4-	0.00000	0,00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
104	MgB(OH)4+	B3O3 (OH) 4-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
301	MgB (OH) 4+	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1 1-2 1-3
- /~e 1 /	MgB (OH) 4+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
5 - S	MgB (OH) 4+	Am (CO3)2- Am (CO3)3=-	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
105	MgB (OH) 4+ MgB (OH) 4+	Am (CO3)3=- ClO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
121	MgB (OH) 4+	NDO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
17:	hgB(OH)4+	Np02C03-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1.1-2.1-3
472	MgB (OH) 4+	Np02 (C03) 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

	- PP		•	_			
		NpO2 (CO3)3=≠-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
	MgB(OH)4+	H2P04~	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
- 7.4	MgB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	(2,0,12) 1-1,1-2,1-3
171	MgB(OH)4+	P04=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
	MgB (OH) 4+		0.12000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
	CaB(OH)4+	C1-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
· 7 2`	CaB (OH) 4+	504=	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
173	CaB (OH) 4+	H504-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
· · · · ·	CaB (OH) 4+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
100	CaB (OH) 4+	HCO3-		0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
137	CaB (OH) 4+	CO3=	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
0	CaB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
	CaB(OH)4+	B303 (OH) 4-	0.00000		0.00000	0.00000	(2.0, 12) $1-1, 1-2, 1-3(2.0, 12)$ $1-1, 1-2, 1-3$
	CaB(OH)4+	B405 (OH) 4≠	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
[A]	CaB (OH) 4+	Br-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
102	CaB (OH) 4+	Am (CO3) 2-	0.00000		0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
102	CaB (OH) 4+	Am (CO3) 3=-	0.00000	0.00000	0.00000	0.000000	(2.0,12) 1-1,1-2,1-3
· <u>-</u> .	CaB (OH) 4+	C104-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
-# `	CaB(OH)4+	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
91	CaB (OH) 4+	Np02C03-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
1 e .	CaB (OH) 4+	NpO2 (CO3) 2=-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
191	CaB(OH)4+	NpO2(CO3)3≠=-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
104	CaB (OH) 4+	H2PO4-	0.00000		0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
10,	CaB(OH)4+	HPO4 =	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
- (4) - (4)	CaB (OH) 4+	P04=-	0.00000	0.00000	0.00000	~0.02840	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
- ú.*	Am+++	C1-	0.61170	5.40300		0.00000	(1.4,50) 2-(n>2)
	Am+++	S04=	3.03980	0.00000	-2500.00000 0.00000	0.00000	(1.4, 50) $2 - (112)(2.0, 12)$ $1 - 1, 1 - 2, 1 - 3$
199	Am+++	HSO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
201	Am+++	OH-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
<u> </u>	Am+++	нсоз -	0.00000		0.00000	0.00000	(1.4,50) 2-(n>2)
	Am+++	CO3≠	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
253	አመ+++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	
23. A	Am+++	B303 (OH) 4-	0.00000	0.00000		0.00000	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
367	Am+++	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	(2.0, 12) $1-1, 1-2, 1-3$
200	Am+++	Br-	0.0000	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		(2.0, 12) 1-1, 1-2, 1-3
	Am+++	Am (CO3)3=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
25 2	Am+++	C104-	0.80000	5.35000	0.00000	-0.00480	(2.0.12) 1-1,1-2,1-3
25	Am+++	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
2	Am+++	Np02C03-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
2.2	Am+++	NpO2 (CO3) 2=-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2- $(n>2)$
	Am+++	NpO2 (CO3) 3==-	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
2.14	Am+++	H2P04-	0.00000	0.00000	-92.90000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
<i>k</i> 0	Am+++	HPO4 =	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2-(n>2)
27.5	Am+++	PO4=-	0.00000	0,00000	0.00000	0.00000	(1.4,50) 2-(n>2)
212	AmCO3+	C1-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
010	AmCO3+	S04=	0.00000	0.00000	D.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
218	AmCO3+	HSO4 -	0.00000	0,00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
22	AmCO3+	OH-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1,1-2,1-3
2.2	AmCO3+	HCO3 -	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	AmCO3+	CO3=	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	AmCO3+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	AmCO3+	B303 (OH) 4-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	AmCO3+	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
228	AmCO3+	Br-	0.00000	0,00000	0.00000	0.00000	(2.0, 12) $1-1, 1-2, 1-3$
<u>///</u>	AmCO3+	Am (CG3)2-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3
	AmCO3+	Am (CO3)3=-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	AmCO3+	C104-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	AmCO3+	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	$\{2.0, 12\}$ 1-1, 1-2, 1-3
	AmCO3+	NpO2CO3-	0.00000	0.00000	0.00000	0.00000	$\{2.0, 12\}$ 1-1, 1-2, 1-3
132	AmCO3+	NpO2 (CO3) 2=-	0.0000.0	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	AmCO3+	NpO2 (CO3) 3==-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
	AmC03+	H2P04-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3
22.5	AmCO3+	HPO4 *	0.00000	0.00000	0.00000	0.00000	(2.0.12) 1-1,1-2,1-3
28) 28)	AmCO3+ Th++++	PO4=~ Cl-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
237	Th++++	S04=	0.00000	0.00000	0.00000	0.00000	
	Th++++			0.00000			(1.4,50) 2-(n>2) (2.0,12) 1-1,1-2,1-3
		HSO4 ~	0.00000	0.00000	0.00000	0.00000	(2.0, 12) $1-1, 1-2, 1-3(2.0, 12)$ $1-1, 1-2, 1-3$
24	Th++++ Th++++	он- нсоз ~	0.00000	0.00000	0.00000	0.00000	(2.0, 12) $1-1, 1-2, 1-3(2.0, 12)$ $1-1, 1-2, 1-3$
		CO3=	0.00000	0.00000	0.00000	0.00000	(1.4,50) 2- $(n>2)$
	Th++++ Th++++		0.00000	0.00000	0.00000	0.00000	(2.0,12) $1-1,1-2,1-3$
		B(OH)4-		0.00000	0.00000	0.00000	
	Th++++ Th++++	B303 (OH) 4-	0.00000				(2.0,12) 1-1,1-2,1-3
		B405 (OH) 4=	0.00000	0.00000	0.00000 0.00000	0.00000	(2.0, 12) 1-1,1-2,1-3
	Th++++ Th++++	Br-	0.00000 0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1,1-2,1-3 (2.0, 12) 1-1,1-2,1-3
		Am(CO3)2-			0.00000		
	Th++++	Am(CO3)3=-	0.00000	0.00000		0.00000	(1.4,50) 2-(n>2)
	Th++++ Th++++	C104~	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (2.0,12) 1-1,1-2,1-3
		NpO2 (OH) 2-	0.00000			0.00000	
	Th++++	Np02003-	0.00000	0.00000	0.00000		(2.0,12) 1-1,1-2,1-3 (1.4,50) 2-(->2)
	Th++++ Th++++	NpO2 (CO3) 2=-	0.00000	0.00000 0.00000	0.00000 0.00000	0.00000	(1.4,50) 2~(n>2) (1.4,50) 2~(n>2)
		NpO2 (CO3) 3==-	0.00000				
	Th++++	H2PO4-	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1-1,1-2,1-3 (1.4,50) 2-(->2)
26í 25e	Th++++ Th++++	HPO4= PO4=-	0.00000.0	0.00000	0.00000	0.00000	(1.4,50) $2 - (n>2)(1.4,50)$ $2 - (n>2)$
	U02++	Cl-		1.64400	0.00000	-0.03686	(1.4,50) 2~(n>2) (2.0,12) 1~1,1-2,1-3
	U02++	S04=	0.42740	1.82700	0.00000	-0.01760	(1.4,12) 2-2
	002++	S04= HS04-	0.32200	0.00000	0.00000	0.00000	
	UQ2++		0.00000				(2.0, 12) $1-1, 1-2, 1-3(2.0, 12)$ $1-1, 1-2, 1-3$
	U02++	OH-	0.00000	0.00000	0.00000	0.00000	(2.0, 12) 1-1, 1-2, 1-3 (2.0, 12) 1-1, 1-2, 1-3
		HCO3 - CO3 =	0.00000	0.00000	0.00000	0.00000	(2.0,12) 1~1,1-2,1-3 (1.4,12) 2~2
262	002++						



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B (OH) 4-B303 (OH) 4-

Br-

B405 (OH) 4=

Am(CO3)2-

Am(CO3)3=-

Np02 (OH) 2-

Np02 (CO3) 2=-

NpO2 (CO3) 3==-

Np02C03-

C104-

H2P04-

HP04 =

P04=-

SO4=

HSO4-

нсоз –

B(OH)4-

B303 (OH) 4-

B405 (OH) 4=

Am (CO3) 2 -

CO3 =

Br-

c1-

OH-

2h3 002++

U02++

U02++

002++

U02++

002++

002++ 222 U02++ 227 U02++ 275 U02++

U02++

NpO2+ 228 NpO2+

NpO2+

NoO2+

Np02+

NpO2+

NDOZ+ 2 Np02+

2 3 002++

28-4 2670 U02++

253

ZU02++

2.5

200 NDO2+

200 NpO2+

Re. Pos NpO2+

204 204 205

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

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NpO2 (OH) 2-

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	NpO2+	Am (CO3) 2 ≁	0.000	
200		Am (CO3)3#-	0.000	
		C104-	0.312	
::00	Np02+	NpO2 (OH) 2-	0.000	
201	NpO2+	Np02C03-	0.000	000 000
200		Np02(C03)2=-	0.000	000 0.00
		Np02 (C03) 3==-		000 0.00
		H2P04-	0.000	000 0.00
		HPO4=	0.000	
		P04=-	0.000	
2.00		104	•••••	
	Cation-Cation 1	Nernens Toters	ctions t	
243		Cetural A mitera		ACCA (C1, C0)
		К+	Ca++	Mg++
340		-0.01200	0.07000	0.07000
	Na+			0.07000
302		U02++	NpO2+	
147	Na+	0.00000	0.0000	
30-		_		
10		Ca++	Mg++	MgOH+
<u> </u>		0.03200	0.00000	0.00000
ಳೆಗಳ		Np02+		
306		0.00000		
339				
(n) (r)		Ng++	MgOH+	H+
211	Ca++	0.00700	0.00000	0.09200
. 3		MgOH+	H+	MgB(OH)4+
- 4	Mg++	0,00000	0.10000	0.00000
210	-			
· · · ·		H+	MaB (OH) 4+	CaB(OH)4+
2.7	MgOH+	0.00000	0.00000	0.00000
\$1 \$				
219		MaB (OH) 4+	CaB(OH)4+	Am+++
327			0.00000	
221				
322		CaB(OH)4+	Am+++	AmC03+
	Mc B (OH) 4+	0.00000		0.00000
3.24				
 		Am+++	AmCO3+	Th++++
	CaB (OH) 4+	0.00000	0.00000	0.00000
327			0.00000	0.00000
22		AmC03+	Th++++	U02++
	Am+++	0.00000	0.00000	0.00000
255	2801111	*	0.00000	0.00000
301		Th++++	002++	NpO2+
	AmCO3+	0.00000	0.00000	0.00000
333	Marcou +	4.00000	0.00000	0.00000
23.2		002++	NpO2+	
	Th++++	0.00000	0.00000	
	.10++++	0.00000	0.00000	
2 × 5				
<u>.</u>	0	NpO2+		
	002++	0.00000		
23.4				
1900				
	Anion-Anion Ter	nary Interact	ions: thet	a(al,a2)
2.43		SO4 =	HSO4 -	OH-
	¢1-			-0.05000
242		Am (CO3)3=-		NpO2 (OH) 2 -
	C1-	0.00000	0.00000	0.00000

1.24

.445 SO4=

32

35: 357

SO4 =

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	K+ -0.01200 U02++	Ca++ 0.07000 NpO2+	Mg++ 0.07000	МgОН+ 0.00000	H+ 0.03600	MgB (OH) 4+ 0.00000	CaB(OH)4+ 0.00000	Am+++ 0.00000	AmCO3+ 0.00000	Th++++ 0.00000
	0.00000	0.00000								
	Ca++ 0.03200 NpO2+ 0.00000	Mg++ 0.00000	MgOH+ 0.00000	₩+ 0.00500	MgB (OH) 4+ 0.00000	CaB(OH)4+ 0.00000	Am+++ 0.00000	AmCO3+ 0.00000	Th++++ 0.00000	UO2++ 0.00000
	Mg++ 0.00700	MgOH+ 0.00000	н+ 0.09200	MgB(OH)4+ 0.00000	CaB(OH)4+ 0.00000	Am+++ 0.00000	AmCO3+ 0.00000	Th++++ 0.00000	0.00000	NpO2+ 0.00000
	MgOH+ 0,00000	H+ 0.10000	MgB(OH)4+ 0.00000	CaB(OH)4+ 0.00000	Am+++ 0.00000	AmCO3+ 0.00000	Th++++ 0.00000	UO2++ 0.00000	NpO2+ 0.00000	
	번+ 0.00000	MgB(OH)4+ 0.00000	CaB(OH)4+ 0.00000	Am+++ 0.00000	AmCO3+ 0.00000	Th++++ 0.00000	UO2++ 0.00000	NpO2+ 0.00000		1
	MgB (OH) 4+ 0.00000	CaB(OH)4+ 0.00000	Am+++ 0.0000	AmCO3+ 0.00000	Th++++ 0.00000	UO2++ 0.00000	Np02+ 0.00000			,
)4+	CaB(OH)4+ 0.00000	Am+++ 0.00000	AmCO3+ 0.00000	Th++++ 0.00000	002++ 0.00000	NpO2+ 0.00000				
) 4+	Am+++ 0.00000	AmCC3+ 0.00000	Th++++ 0.00000	002++ 0.00000	NpO2+ 0.00000				,	م مراجع ا
	AmCO3+ 0.00000	Th++++ 0.00000	0.00000	NpO2+ 0.00000						
	Th++++ 0.00600	0.00000	NpO2+ 0.00000							
	0.00000	NpO2+ 0.00000								
	NpO2+ 0.00000									
Anion Te	rnary Interact	ions: thet	a(a1,a2)							
	SO4≠ 0.02000 Am(CO3)3=- 0.00000	HS04- -0.00600 C104- 0.00000	ОН- -0.05000 NpO2(ОН)2- 0.00000			B(OH)4- -0.06500 NpO2(CO3)3 0.00000	0.12000	B405 (0H) 4= 0.07400 HP04= 0.00000	Br- 0.00000 PO4=- 0.00000	Am (CO3) 2- 0.00000
	H504- 0.00000	ОН- ~0.01300	HCO3 - 0.01000	CO3= 0.02000	B(OH)4-	B303 (OH) 4~ 0.10000	B4O5 (OH) 4≃ 0.12000	Br- 0.00000	Am (CO3)2~ 0.00000	Am (CO3)3≠- 0.00000

Np02(C03)2 Np02(C03)3 H2P04-

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HPO4=

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(1.4,50) 2-(n>2) (2.0,12) 1-1,1-2,1-3

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(2.0,12) 1-1,1-2,1-3

(2.0,12) 1-1,1-2,1-3

(1.4.50) 2-(n>2)

(1.4,50) 2-(n>2)

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•	-pp-ment of a		•								
555	H504-	ОН- 0.00000 NPO2 (ОН) 2-	HCO3 - 0.00000 NpO2CO3- 0.00000	CO3= 0.00000 NpO2(CO3)2 0.00000	B(OH)4+ 0.00000 NpO2(CO3)3 0.00000	0,00000	B405 (OH) 4= 0,00000 RP04= 0,00000	= Br- 0.00000 PO4=- 0.00000	Am (CO3)2- 0.00000	Am(CO3)3=- 0 00000	C104- 0.00000
225	HSO4-	0.00000 HCO3-	C03=	B(OH)4-	B303 (OH) 4-			Am (CO3)2-	Am (CO3)3=-	C104-	Np02(0H)2-
154 44 2 (m. 2	OH-	0.00000 Np02C03+	0.10000	0.00000 NpO2 (CO3) 3	0.00000	0.00000 HPO4=	0.00000 PO4=-	0.00000	0.00000	0,00000	0.0000
	ОН-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000				
36. 31 44	HCO3-	CO3= -0.04000 NpO2(CO3)2 0.00000	B(OH)4- 0.00000 NDO2(CO3)3 0.00000	-0.10000	B405 (OH) 4= -0.08700 HPO4= 0.00000	Br- 0.00000 PO4=- 0.00000	Am (CO3)2- 0.00000	Am (CO3)3≂– 0.00000	C104- 0.00000	N702 (0H)2- 0.00000	NpO2CO3- 0.00000
267 200	co3=	B(OH)4- 0.00000		B405 (OH) 4=		Am(CO3)2-	Am (CO3)3= 0.00000	- C104- 0.00000	NpO2 (ОН) 2 - 0.00000	Np02C03- 0.00000	NpO2 (CO3) 2
473) 275	co3=	NpO2 (CO3)3 0.00000		HPO4= 0.00000	PO4=- 0.00000						
273 374 378	в (ОН) 4-	0.00000 H2P04-	B405 (OH) 4= 0.00000 HP04=	0.00000 PO4=-	Am (CO3)2+ 0.00000	Am (CO3)3≉- 0.00000	0.00000	NpO2 (OH) 2- 0.00000	NpO2CO3- 0.00000	NpO2(CO3)2 0.00000	NpO2(CO3)3 0.00000
377	B(OH)4-	0.00000	0.00000	0.00000							
	B3O3 (OH) 4~ B3O3 (OH) 4-	B405(DH)4= 0.00000 HP04= 0.00000	Br- 0.00000 PO4=- 0.00000	Am (CO3)2- 0.00000	Am (CO3)3=- 0.00000	C104- 0.00000	NpO2 (0H) 2 0.00000	- Np02C03- 0.00000	NpO2 (CO3) 2 0.00000	NDO2 (CO3)3 C.00000	H2P04- 0.00000
2012 (2013	8303 (04/4-	Br-	Am(C03)2-	Am(CO3)3=-	C104-	NpO2 (OH) 2-	ND02C03-	ND02 (C03) 2	Np02 (003) 3	F2P04-	HP04=
243 201	B4Q5 (OH) 4=	0.00000 PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	¢.00000	0.0000
	B4O5 (OH) 4=	0.00000									
19892 2850 2850	Br-	Am (CO3)2- 0.00000	Am (CO3)3=- 0.00000	C104- 0.00000	NpO2(OH)2- 0.00000	NpO2CO3- 0.00000	NpO2 (CO3): 0.00000	2 NpO2(CO3)3 0.00000	H2PO4- 0.00000	HP04= 0.00000	PO4=- 0.00000
201	Am (CO3)2~	Amr(CO3)3≖– 0.00000	C104- 0.00000	NpO2(OH)2- 0.00000	Np02003- 0.00000	NpO2 (CO3)2 0.00000	2 NpO2 (CO3) 0.00000	3 H2PO4- 0.00000	HPO4 = 0.00000	PO4=- 0.00000	
5	Am (CO3)3≈-	C104- 0.00000	NpO2(OH)2- 0.00000	Np02C03~ 0.00000	NpO2(CO3)2 0.00000	NpO2 (CO3)3 0.00000	H2PO4- 0.00000	HPC4= 0.00000	PO4=- 0.00000		
202 208 306	C104-	Np02 (OH) 2- 0.00000	Np02C03- 0.00000	NpO2(CO3)2 0.00000	NCO2 (CO3) 3 0.00000	H2P04- 0.00000	HP04= 0.00000	PO4=- 0.00000			
400	Np02 (OH) 2-	Np02C03- 0.00000	NpO2(CO3)2 0,00000	NpO2 (CO3) 3 0.00000	H2PO4- 0.00000	HPO4= 0.00000	PO4=- 0.00000				
~0°;	Np02C03-	Np02(C03)2 0.00000	NpO2(CO3)3 0.00000	H2P04- 0.00000	нро4= 0.00000	PO4≃- 0.0000D					
<u>.</u>	NpO2(C03)2=-	NpO2 (CO3)3 0,00000	H2PO4- 0.00000	HPO4# 0.00000	PO4=- 0.00000						S. S. C.
61 a	Np02 (CO3) 3==-	H2PO4- 0.00000	NPO4= 0.00000	PO4=- 0.00000							
273) 414	H2P04-	HPO4= 0.00000	PO4=- 0.00000								· · ·
410 410 217	HPO4=	PO4=- 0.00000	4								•
458 413 442	Cation-Cation-A	nion Ternary	Interaction	s: psi(,,,	}						
		••	C1-	SO4=						(OH)4 B405 (
422		K+ Ca++	-0.00180 -0.00700	-0.01000 -0.05500					0000 0.00		
674		Mg++	-0.01200	-0.01500					0000 0.00		
120	Na+	МдОң+	0.00000	0.00000	0.00000		,00000 0	.00000 0.0	0000 0.00	000 0.000	00 0.00000
4.20		H+	-0.00400						0000 0.00		
		MgB(OH)4+	0.00000	0.00000					0000 0.00		
423) 429		CaB (OH) 4+ Am+++	0.00000	0.00000.0					0000 0.00 0000 0.00		
		AmCQ3+	0.00000	0.00000					0000 0.00		
		Th++++	0.00000	0.00000	0.00000	0.00000 0	0.00000 0	.00000 0.0	0000 0.00	000 0.000	00 0.00000
		002++	0.00000	0.00000					0000 0.00		
		NpO2+	0.00000	0.00000					0000 0.00		
-34 101		Ca++ Mg++	-0.02500 -0.02200	0.00000					0000 0.00		
1.0		MgOH+	0.00000	0.00000					0000 0.00		
6.57		H+	-0.01100	0.19700	~0.02650	0.00000 0	0.00000 0	,00000 0.0	0000 0.00	000 0.000	00 0.00000
رئو به	K+	MgB (OH) 4+	0.00000	0.00000	0.0000	0.00000 (0 00000,0	.00000 0.0	0000 0.00	000 0.000	00 0.00000
~: 		CaB(OH)4+	0.00000	0.00000					0000 0.00		
44(34)		Am+++ AmC03+	0.00000	0.00000 0.00000					0000 0.00		
663		Th++++	0.00000	0.00000					0000 0.00		

los K+ ⊷ K+	002++ Np02+	0.00000	0.00000	0.00000.0	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
5 Ca++	Mg++	-0.01200	0.02400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
Ca++	MgOH+		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	D.000
; Ca++	H+	-0.01500			0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.000
: Ca++	MgB (OH) 4+	0.0000	0.00000	0.00000							
3 Ca++	CaB(OH)4+	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
Ca++	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
* Ca++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000	0.00000	0.000
2. Ca++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Ca++	002++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
		0.02800	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.00
⊙ Mg++	MgOH+		0.00000	-0.01780	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
-> Mg++	H+	-0.01100					0.00000	0.00000	0.00000	0.00000	0.00
,? Mg++	MgB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000					
🖄 Mg++	CaB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
a Mg++	እመ+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00
Mg++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Mg++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
-	U02++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Mg++				0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
🔆 Mg++	NpO2+	0.00000	0.00000								
😳 MgOH+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
MgOH+	MgB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
MgOH+	CaB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
MgOH+	Am+++	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000.0	0.00000	0.00000	0.00
-		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.00
MgOH+	AmCO3+			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
MgOH+	Th++++	0.00000	0.00000								
MgOH+	002++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
MgOH+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Э. н.	MgB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
С н+	CaB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
- H+	Am+++	0.00000	0.00000	0.00000.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0,00000	0,00000	0.00
			0,00000			0.00000	0.00000	0.00000	0.00000	0.00000	0.00
С н+	Th++++	0.00000		0.00000	0.00000						
" н+	U02++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
`` H+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
9 MgB (OH) 4+	CaB (OH) 4+	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
MgB (OH) 4+	Am+++	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
MgB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
2. MgB(OH)4+	772++++										
8 MgB (OH) 4+	U02++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
∽ MgB{OH}4+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
🔆 CaB (OH) 4+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
-> CaB (OH) 4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
CaB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
				0.00000	0.00000	0.00000	0.00000	0.00000	0,00000	0,00000	0.00
⊙ СаВ (ОН) 4+	NpO2+	0.00000	0.00000								
🔆 Am+++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000	0.00
4 Am+++	Th++++	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Am+++	UO2++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Am+++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
AmCO3+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
AmCO3+	002++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000.0	0.00000	0.00
AmCO3+	Np0.2+	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000	0.0000	0.00000	0.00
° Th++++	002++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
5 Th+++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
℃ UO2++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
:	-										
:		Am(00332-	- Am (CO3) 3=	- C104-	Np02 (OH) 2	Nn02C03 -	Np02 (C03)	Np02 (CO3)	H2P04-	HP04=	P04=
	K+		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0,00000	0.00
		0.00000		0.00000							
Na+	Ca++	0.00000	0.00000		0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00
- Na+	Mg++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000	0.00000	0.00000	0.00
Na+	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
S Na+	H+	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
: Na+	MgB (CH) 4+	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Na+	CaB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Na+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000	0.00000		
										0.00000	0.00
Na+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Na+	002++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Na+	Np02+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
- K+	Ca++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
. K+	Mg++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
, K+	MgOH+	0.00000	0.00000	0.000000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
											0.00
	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
č K+	MgB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
× K+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
. K+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
K+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
K+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	002++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
: К+	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
K+	Mg++	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
K+	MgOH+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
4 K+ Ca++			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
′ K+ └ Ca++ ℃ Ca++	H+									0.00000	
4 K+ € Ca++ € Ca++ 7 Ca++	H+ M=P (OV) A+	0.00000		0 00000	0 00000	0 00000	<u>n nnnnn</u>	A AAAAA	0 00000	A 66444	· · · ·
⁴ K+ ³ Ca++ ² Ca++ ² Ca++ ³ Ca++	Mg8 (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
 K+ Ca++ Ca++ Ca++ Ca++ Ca++ Ca++ 	Mg8 (ОН) 4+ СаВ (ОН) 4+	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
4 K+ 5 Ca++ 7 Ca++ 9 Ca++ 5 Ca++ 5 Ca++ 1 Ca++	Mg8 (OH) 4+	0.00000	0.00000								0.00
4 K+ 5 Ca++ 7 Ca++ 7 Ca++ 7 Ca++ 5 Ca++	Mg8 (ОН) 4+ СаВ (ОН) 4+	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00 0.00 0.00

...

	Appendix J: V											
	_		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	Ca++	002++ אסטקא	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
С. 534	Ca++ Ma++	MgOH+	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	D.00000	0.00000	0.00000
330	Mg++ Mg++	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
53	Mg++	MgB (OH) 4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.52	Mg++	CaB (OH) 4+	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000
5 N.	Mg++	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-	Mg++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2.4	Mg++	Th++++	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-12	Mg++	002++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000)	0.00000	0.00000
511	Mg++	Np02+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
the second	MgOH+	H+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	MgOH+ MgOH+	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
, -4-) 1	MgOH+	Am+++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
545	MgOH+	AmCO3+	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
545	MgOH+	Tn++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
35	MgOH+	002++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
\$14 X	MgOH+	Np02+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
14 B.M	H+	MgB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.13	H+	CaB(OH)4+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000
-96. -	H-	Am+++	0.00000 0.00000	0.00000	0.00000 0.00000	0,00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000
30). S	위+ H+	AmCO3+ Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	H+	U02++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	H+	NpO2+	0.00000	0.00000	0.0000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
÷54	MgB(OH)4+	CaB (OH) 4+	0.00000	0.00000	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	MgB(OH)4+	Am+++	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5C I	MgB(OH)4+	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
54.2	MgB (OH) 4+	772++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
26	MgB(OH)4+	U02++	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000.0 00000.0
	MgB(OH)4+	Np02+ Am+++	0.00000.0	0.00000	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
507 500	CaB(OH)4+ CaB(OH)4+	Amero3+	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
507	CaB(OH)4+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
545	CaB(OH)4+	U02++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
- S - S	CaB (OH) 4+	Np02+	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000
<u>.</u>	Am+++	AmCO3+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
. 7	Am+++	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
472.	Am+++	002++	0.00000	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
373	Am+++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	AmCO3+	Th++++	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
575 575	AmCO3+ AmCO3+	U02++ Np02+	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	Th++++	U02++	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
373	Th++++	NpO2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
572	U02++	Np02+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
52.5												
[h]	Anion-Anion-Ca											
		ation Ternary In	teractions	: psi(,,,)							
		ation Ternary In				Maria	N-014-	N.	N-D (OU) 44	- C-B (01) (4		N=203+
500		_	Na+	X+	Ca++	Mg++ -0.00400	мдО∺+ 0.00000	H+		- CaB (OH) 44		AmCO3+
500 554	c1-	SO4=	Na+ 0.00140	X≁ 0.00000	<i>Ca++</i> -0.01800	-9.00400	0.00000	0.00000	0.00000	0.0000.0	0.00000	0.00000.0
500		_	Na+	X+	Ca++							
500 554 565	C1- C1-	504= HS04-	Na+ 0.00140 -0.00600	X+ 0.00000 0.00000 -0.00600 0.00000	Ca++ -0.01800 0.00000 ~0.02500 0.00000	-0.00400 0.00000	0,00000	0.00000	0.00000 0.00000 0.00000 0.00000	0.0000.0	0.00000	0.00000 0.00000
	C1- C1- C1- C1- C1-	SO4 = HSO4 - OH- HCO3 - CO3 =	Na+ 0.00140 -0.00600 -0.00600 -0.01500 0.00850	X+ 0.00000 -0.00000 -0.00600 0.00000 0.00400	Ca++ -0.01800 0.00000 -0.02500 0.00000 0.00000	-0.00400 0.00000 0.00000 -0.09600 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	03000.0 03000.0 03000.0 03000.0	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000
	C1- C1- C1- C1- C1- C1-	SO4 = HSO4 - OH - HCO3 - CO3 = B (OH) 4 -	Na+ 0.00140 -0.00600 -0.00600 -0.01500 0.00850 -0.00730	X+ 0.00000 -0.00000 -0.00000 0.00000 0.00400 0.00000	Ca++ -0.01800 0.00000 -0.02500 0.00000 0.00000 0.00000	-0.00400 0.00000 0.00000 -0.09600 0.00000 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	03000.0 03000.0 03000.0 03000.0 03000.0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	c1- c1- c1- c1- c1- c1- c1- c1-	SO4 = HSO4- OH- HCO3- CO3= B (OH)4- B3O3 (OH)4-	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 -0.02400	X+ 0.00000 -0.00000 0.00000 0.00000 0.00400 0.00000 0.00000	Ca++ -0.01800 0.00000 -0.02500 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 0.00000 -0.09600 0.00000 0.00000 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	03000.0 03000.0 03000.0 03000.0 03000.0 03000.0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	C1- C1- C1- C1- C1- C1- C1- C1-	SO4 = HSO4 - OH - HCO3 - CO3 = B(OR)4 - B3O3(OH)4 - B4O5(OR)4 =	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 -0.02400 0.02600	X+ 0.00000 -0.00000 0.00000 0.00400 0.00000 0.00000 0.00000	Ca++ -0.01800 -0.02500 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	03000.0 03000.0 03000.0 03000.0 03000.0 03000.0 03000.0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	c1- c1- c1- c1- c1- c1- c1- c1-	SO4 = HSO4- OH- HCO3- CO3 = B (OH) 4- B3O3 (OH) 4- B4O5 (OH) 4= Br-	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 -0.02400 0.02600 0.02600	X+ 0.00000 -0.00000 0.00000 0.00000 0.00400 0.00000 0.00000	Ca++ -0.01800 0.00000 -0.02500 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 0.00000 -0.09600 0.00000 0.00000 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	00000.0 0000.0 0000.0 00000.0 00000.0 00000.0 00000.0 00000.0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	C1- C1- C1- C1- C1- C1- C1- C1- C1- C1-	SO4 = HSO4 - OH - HCO3 - CO3 = B(OR)4 - B3O3(OH)4 - B4O5(OR)4 =	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 -0.02400 0.02600	X+ 0.00000 0.00000 0.00000 0.00400 0.00400 0.00000 0.00000 0.00000 0.00000	Ca++ -0.01800 0.00000 -0.02500 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	03000.0 03000.0 03000.0 03000.0 03000.0 03000.0 03000.0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4 - OH - HCO3 - CO3 = B(OH) 4 - B4O5(OH) 4 - B4O5(OH) 4 = Br - Am(CO3) 2 - Am(CO3) 2 - Am(CO3) 2 -	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 -0.02400 0.02600 0.00000 0.00000 0.00000	X+ 0.00000 0.00000 0.00000 0.00400 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Ca++ -0.01800 0.0000 -0.02500 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.00600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4 - OH - HCO3 - CO3 = B(OH) 4 - B3O3(OH) 4 - B4O5(OH) 4 - BT - Am(CO3) 2 - Am(CO3) 2 - Am(CO3) 3 = - C1O4 - NpO2(OH) 2 -	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02400 0.02400 0.00000 0.00000 0.00000 0.00000	X+ 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Ca++ -0.01800 -0.02500 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.09500 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- 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 - NpO2 (O3 -	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.023400 0.02600 0.02600 0.00000 0.00000 0.00000 0.00000 0.00000	X+ 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	Ca++ -0.01800 0.00200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000 0.00000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B4O5(OH)4- B4O5(OH)4- Br- Am(CO3)3=- C104- NpO2(OH)2- NpO2(CO3)2=-	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 -0.02400 0.02600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	X+ 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Ca++ -0.01800 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.0000 0.01300 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	C1-	SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)3==-	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02400 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	X+ 0.00000 -0.00600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Ca++ -0.01800 0.00000 -0.02500 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0,00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.000000 0.00000 0.000000 0.000000 0.000000 0.00000000
	Cl- Cl- </th <th>SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- C1O4- NpO2(OH)2- NpO2(CO3)3=- NpO2(CO3)3=- H2PO4-</th> <th>Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 0.02400 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000</th> <th>X+ 0.00000 0.000000 0.000000 0.000000 0.000000 0.0000000 0.000000 0.00000000</th> <th>Ca++ -0.01800 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000</th> <th>-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000</th> <th>0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000</th> <th>0.0000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000</th> <th>0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000</th> <th>0 2000.0 0 200.</th> <th>0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000</th> <th>0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000</th>	SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- C1O4- NpO2(OH)2- NpO2(CO3)3=- NpO2(CO3)3=- H2PO4-	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 0.02400 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	X+ 0.00000 0.000000 0.000000 0.000000 0.000000 0.0000000 0.000000 0.00000000	Ca++ -0.01800 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	C1-	SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)3==-	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02400 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	X+ 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Ca++ -0.01800 0.00000 -0.02500 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0,00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.000000 0.00000 0.000000 0.000000 0.000000 0.00000000
22日本部での12月前になった。19月前の19月1日	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B4O5(OH)4- B4O5(OH)4- Br- Am(CO3)3- ClO4- NpO2(OH)2- NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)3==- H2PO4- HPO4=	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02600 0.02600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	X+ C.00000 C.00600 C.00400 C.00400 C.000000 C.00000 C.000000 C.000000 C.000000 C.000000 C.000000 C.00000 C.00000 C.00000	Ca++ -0.01800 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4- OH- HCO3- CO3= B(OR)4- B3O3(OH)4- B4O5(OR)4= B4O5(OR)4= Br- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OH)2- NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)3==- HPO4= HPO4= HSO4- OH-	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02400 0.02600 0.000000	X+ C.00000 C.00600 C.00400 C.000000 C.000000 C.0000000 C.000000 C.000000 C.00000 C.00000 C	Ca++ -0.01800 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.0000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
の社会会になったのでありのでのつうなどのです。	C1- C1- C1- C1- C1- C1- C1- C1-	SO4 = HSO4- OH- HCO3- CO3= B(OR)4- B3O3(OH)4- B4O5(OR)4- B4O5(OR)4- Br- Am(CO3)2- Am(CO3)3=- C104- NpO2(OA)2- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- H2O4- H2O4= H2O4= H2O4= H2O4= H2O4= H2O4= OH-	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02400 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 -0.00940 -0.00500	X+ 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.00000000	Ca++ -0.01800 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.00000 -0.09600 0.00000	0,00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- 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- NpO2(OH)2- NpO2(CO3)3=- H2PO4- H2PO4= HSO4- OH- HCO3- CO3=	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 -0.00940 -0.00500	X+ 0.000000 0.0000000 0.000000 0.000000 0.000000 0.00000000	Ca++ -0.01800 0.00200 0.02500 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 -0.04250 0.00000 -0.16100 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000000
2013年1月1日、1月1日、1月1日、1月1日、1月1日、1月1日、1月1日、1月1日	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4= HSO4- OH- HCO3- CO3= B(OE)4- B3O3(OH)4- B4O5(OE)4= B4O5(OE)4= BT- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OG)3=- ClO4- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- H2PO4- H2PO4=- H2PO4=- HSO4- OH- HCO3- CO3= B(OH)4-	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.02300 0.02600 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00500 -0.00500 0.00500	X+ C.50000 D.00000 C.00000 C.00000 D.00000 D.00000 D.00000 C.000000 C.0000000 C.000000 C.000000 C.00000 C.00000 C.00000 C.	Ca++ -0.01800 0.000000 0.00000 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.16100 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.0000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.000000 0.00000 0.000000 0.000000 0.00000000
	C1- C1- C1- C1- C1- C1- C1- C1-	SQ4 = HSQ4- OH- HCQ3- CQ3= B(OH)4- B3Q3(OH)4- B4Q5(OH)4- B4Q5(OH)4- B4Q5(OH)4- MpQ2(OH)2- NpQ2(CQ3)3=- ClQ4- NpQ2(CQ3)3=- HPQ4- HPQ4= HPQ4= HPQ4= HPQ4= HSQ4- OH- HCQ3- CQ3= B(OH)4- B3Q3(OH)4-	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02600 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00940 -0.00940 -0.00940 -0.00900 0.00000 0.00000	X+ C. D0000 C. 00600 C. 00600 C. 00000 C. 00000 C	Ca++ -0.01800 0.000000 0.00000 0.000000 0.000000 0.00000000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 -0.04250 0.00000 0.00000 -0.16100 0.00000	C.00000 C.000000 C.000	0.00000 0.01300 0.00000	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 20000 0 0 2000 0 0 200	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.000000 0.00000 0.000000 0.000000 0.00000000
2013年1月1日、1月1日、1月1日、1月1日、1月1日、1月1日、1月1日、1月1日	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4= HSO4- OH- HCO3- CO3= B(OE)4- B3O3(OH)4- B4O5(OE)4= B4O5(OE)4= BT- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OG)3=- ClO4- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- H2PO4- H2PO4=- H2PO4=- HSO4- OH- HCO3- CO3= B(OH)4-	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.02300 0.02600 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00500 -0.00500 0.00500	X+ C.50000 D.00000 C.00000 C.00000 D.00000 D.00000 D.00000 C.000000 C.0000000 C.000000 C.000000 C.00000 C.00000 C.00000 C.	Ca++ -0.01800 0.000000 0.00000 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 -0.16100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000 0,00000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.000000 0.00000000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- 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- NpO2(OH)2- NpO2(CO3)3=- H2PO4- H2PO4= H2PO4= HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B3O3(OH)4=	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.00730 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 -0.00940 -0.00500 -0.00500 0.00000 0.00000 0.00000	X+ 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.00000000	Ca++ -0.01800 0.0000 0.02500 0.000000 0.000000 0.00000000	-0.00400 0.00000 -0.09600 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 -0.04250 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0,00000 0,00000	0.00000 0.01300 0.00000	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 20000 0 0 2000 0 0 200	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.000000 0.00000 0.000000 0.000000 0.00000000
2014年1月1日、1月1日、1月1日、1月1日、1月1日、1月1日、1月1日、1月1日	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4- OH- HCO3- CO3= B(OE)4- B3O3(OE)4- B3O3(OE)4- B4O5(OE)4* Br- Am(CO3)2- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OE)3=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- H2PO4- H2PO4- H2PO4- H2PO4- H2PO4- H2PO4- H2PO4- H2PO4- H2PO4- B3O3(OE)	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.02300 0.02600 0.02000 0.00000	<pre>X+ C.50000 O.00000 O.00000 O.00000 O.00000 O.00000 O.00000 C.00000 C.00000 C.00000 C.00000 O.00000 C.00000 C.00000 C.00000 C.00000 C.00000 C.00000 C.00000 O.00000 C.000000 C.00</pre>	Ca++ -0.01800 0.000000 0.00000 0.00000 0.000000 0.000000 0.00000000	-0.00400 0.00000	0.00000 0.000000	0.00000 0.01300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 2000.0 0 200.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.000000 0.000000 0.000000 0.00000000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B3O3(OH)4- B3O3(OH)4- B4O5(OH)4* Br- Am(CO3)2- Am(CO3)2=- NpO2(OH)2- NpO2(OH)2- NpO2(CO3)2=- H2PO4- H2PO4- H2PO4- H2PO4- H2PO4- HSO4- OH- HCO3- CO3- CO3- B(OH)4- B3O3(OH)4- B3O3(OH)4- B3O3(COA)2- Am(CO3)2- Am(C	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.023400 0.02600 0.000000	<pre>X+ C.00000 O.00000 O.00000 O.00000 O.00000 O.00000 O.00000 C.000000 C.00</pre>	Ca++ -0.01800 0.000000 0.00000 0.00000 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.00000	0.00000 0.00000	0.00000 0.01300 0.00000	0.0000 0.00000 0.000000 0.00000 0.00000 0.00000 0.000000 0.00000000	0 20000 0 0 2000 0 0 200	0.00000 0.00000	0.00000 0.000000 0.000000 0.000000 0.00000000
	C1- C1- C1- C1- C1- C1- C1- C1-	SO4 = HSO4 - OH - HSO4 - OH - HSO4 - OH - HSO3 - CO3 = B(OH) 4 - B3O3(OH) 4 - B4O5(OH) 4 - B4O5(OH) 4 - B4O5(OH) 4 - B4O5(OH) 2 - NpO2(CO3) 3 = - C1O4 - NpO2(CO3) 3 = - H2PO4 - HSO4 - OH - HSO4 - OH - HSO4 - OH - HSO4 - OH - HSO3 - CO3 = B(OH) 4 - B3O3(OH) 4 - B3	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02400 0.02000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00940 -0.00000 -0.00000 -0.00940 -0.00940 -0.00000 -0.00000 -0.00940 -0.00940 -0.00000 -0.00000 -0.00940 -0.00000 -0.00000 -0.00940 -0.00000 -0.00000 -0.00000 -0.00940 -0.000000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000000	<pre>X+ C.00000 O.00000 C.00400 C.00000 O.00000 O.00000 C.000000 C.00</pre>	-0.01800 0.02500 0.000000 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.000000	C. 00000 C. 000000 C. 00000 C. 00000000 C. 0000000 C. 000000 C. 0000000000	0.00000 0.01300 0.000000	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 20000 0 0 2000 0 0 200	0.00000 0.000000 0.000000 0.000000 0.00000000	0.00000 0.00000000
2018年1月1日、1月1日、1月1日日に1月1日、1月1日、1月1日、1月1日、1月1日	C1- C1- C1- C1- C1- C1- C1- C1-	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- NpO2(OH)2- NpO2(CO3)3=- H2PO4- H2PO4= H2PO4= H2PO4= H2PO4= HSO4- OH- HCO3- CCO3= B(OH)4- B3O3(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OH)2- N	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.02300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 -0.00500 -0.00500 0.00000	X+ 0.000000 0.000000 0.000000 0.00000000	Ca++ -0.01800 0.0000 0.02500 0.00000 0	-0.00400 0.00000 -0.09600 0.000000	C.00000 C.0000	0.00000 0.01300 0.000000	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 2000.0 0 200.	0.00000 0.00000	0.00000 0.000000 0.000000 0.000000 0.00000000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)2=- HSO4- OH- HSO4- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND04-	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.023400 0.02400 0.02000 0.00000	<pre>X+ C.50000 O.00000 O.00000 O.00000 O.00000 O.00000 O.00000 C.000</pre>	Ca++ -0.01800 0.0000 0.00000 0	-0.00400 0.00000 -0.00000 0.00000	0.00000 0.000000	0.00000 0.01300 0.000000	0.0000 0.00000 0.0000000 0.000000 0.000000 0.00000000	0 2000.0 0 200.	0.00000 0.000000	0.00000 0.00000000
	C1- C1- C1- C1- C1- C1- C1- C1-	SO4 = HSO4- OH- HCO3- CCO3= B(OR)4- B3O3(OH)4- B4O5(OR)4= B4O5(OR)4= Br- Am(CCO3)3=- ClO4- NpO2(OC)33=- ClO4- NpO2(CO3)2=- NpO2(CCO3)3==- HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4-	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02400 0.02000 0.000000	<pre>X+ C.00000 O.00000 C.00400 O.00000 O.00000 O.00000 O.00000 C.000000 C.00000 C.00000 C.00000 C.00000 C.00000 C.00000 C.00000 C.00</pre>	-0.01800 0.02500 0.000000 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.000000	C. 00000 C. 000000 C. 00000000 C. 000000 C. 000000 C. 00000 C. 00000 C. 000	0.00000 0.01300 0.000000	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 20000 0 0 2000 0 0 200	0.00000 0.000000 0.000000 0.000000 0.00000000	0.00000 0.000000 0.00000 0.00000 0.00000 0.0000000 0.000000 0.000000 0.000000 0.00000 0.00000 0.00000 0.0000
	Cl- Cl- Cl- Cl- Cl- Cl- Cl- Cl-	SO4 = HSO4- OH- HCO3- CO3= B(OH)4- B3O3(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)2=- HSO4- OH- HSO4- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND02(OH)2- ND04-	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.02300 0.00000	X+ 0.000000 0.000000 0.000000 0.000000 0.00000000	Ca++ -0.01800 0.0000 0.02500 0.000000	-0.00400 0.00000	C.00000 C.000000 C.000000 C.00000 C.00000000	0.00000 0.01300 0.000000	0.00000 0.000000	0 2000.0 0 200.	0.00000 0.00000	0.00000 0.000000 0.000000 0.000000 0.00000000
2018年1月1日、1月1日、1月1日日、1月1日、1月1日、1月1日、1月1日、1月1	C1- C1- C1- C1- C1- C1- C1- C1-	$\begin{array}{l} SO4 = \\ HSO4 - \\ OH- \\ HCO3 - \\ CO3 = \\ B(OH) 4 - \\ B3O3 (OH) 4 - \\ B4O5 (OH) 4 - \\ D100 (OH) 2 - \\ NpO2 (O3) 3 = - \\ ClO4 - \\ NpO2 (CO3) 2 - \\ NpO2 (OH) 4 - \\ B3O3 (OH) 4 - \\ B4O5 (OH) 4 - \\ B4O5 (OH) 4 - \\ BT - \\ Am (CO3) 2 - \\ Am (CO3) 2 - \\ NpO2 (OH) 2 - \\ NpO2 (OH) 2 - \\ NpO2 (CO3) 2 - \\ NpO3 (CO3) 2 - \\ N$	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02400 0.02400 0.02000 0.000000	<pre>X+ C.00000 O.00000 C.00400 O.00000 O.00000 O.00000 O.00000 C.000000 C.00000 C.00000 C.00000 C.00000 C.00000 C.00000 C.00000 C.00</pre>	-0.01800 0.02500 0.000000 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.000000	C.00000 C.0000	0.00000 0.01300 0.000000	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0 20000 0 0 2000 0 0 200	0.00000 0.000000 0.000000 0.000000 0.00000000	0.00000 0.000000 0.00000 0.00000 0.00000 0.0000000 0.000000 0.000000 0.000000 0.00000 0.00000 0.00000 0.0000
2.855.555.222.855.255.858.8555.201.828.458.458.458.457.4111.1111.1111.1111.1111.11111.11111.1111	C1- C1- C1- C1- C1- C1- C1- C1-	$\begin{array}{l} SO4 = \\ HSO4 - \\ OH- \\ HCO3 - \\ CO3 = \\ B(OH) 4 - \\ B3O3 (OH) 4 - \\ B4O5 (OH) 4 - \\ D700 (CO3) 3 - \\ ClO4 - \\ NpO2 (CO3) 3 - \\ ClO4 - \\ NpO2 (CO3) 3 - \\ NpO2 (CO3) 2 - \\ NpO2 (CO3) 3 - \\ NpO2 (CO3) 3 - \\ ClO4 - \\ NpO2 (CO3) 3 - \\ ClO4 - \\ HSO4 - \\ OH - \\ HSO4 - \\ OH - \\ HSO4 - \\ OH - \\ CO3 - \\ NpO2 (OH) 4 - \\ Br - \\ Am (CO3) 2 - \\ NpO2 (OH) 2 - \\ NpO2 (CO3) 2 - \\ NpO3 (CO3) 2 - \\ Np$	Na+ 0.00140 -0.00600 -0.01500 0.00850 -0.02300 0.02600 0.00000	<pre>X+ C.50000 O.00000 O.00000 O.00000 O.00000 O.00000 C.000000 C.000000 C.00000000</pre>	Ca++ -0.01800 0.00000	-0.00400 0.00000 -0.09600 0.000000	0.00000 0.000000	0.00000 0.01300 0.00000	0.0000 0.00000 0.000000	0 2000.0 0 200.	0.00000 0.000000	0.00000 0.00000000
2.855.555.222.855.255.858.8555.201.828.458.458.458.457.4111.1111.1111.1111.1111.11111.11111.1111	C1- C1- C1- C1- C1- C1- C1- C1-	$\begin{array}{l} SO4 = \\ HS04 - \\ OH - \\ HC03 - \\ CO3 = \\ B(OR)4 - \\ B3O3(OH)4 - \\ B4O5(OR)4 + \\ Br - \\ Am(CO3)2 - \\ Am(CO3)2 - \\ Am(CO3)3 = - \\ Cl04 - \\ NpO2(OH)2 - \\ NpO2(O3)2 - \\ NpO2(O3)2 - \\ NpO2(CO3)2 - \\ NpO2(CO3)2 - \\ NpO2(CO3)2 - \\ NpO2(CO3)2 - \\ HPO4 - \\ HPO4 - \\ HC03 - \\ CO3 - \\ B1O4 - \\ HPO4 - \\ HO4 - \\ HPO4 -$	N2+ 0.00140 -0.00600 -0.01500 0.00850 -0.02300 0.02400 0.02000 0.00000	<pre>X+ C.00000 O.00000 O.00000 O.00000 O.00000 O.00000 O.00000 C.000000 C.000000 C.00000000</pre>	-0.01800 0.02500 0.000000 0.000000 0.000000 0.000000 0.00000000	-0.00400 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000	C.00000 C.0000		0.0000 0.00000 0.0000000 0.000000 0.000000 0.00000000	0 20000 0 0 2000 0 0 200	0.00000 0.000000 0.000000 0.000000 0.00000000	0.00000 0.000000 0.00000000

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

	Appendix 1.	OUTFOI ME	Disting of	· · · · · · · · · · · · · · · · · · ·								
(2)	H504-	CO3 =	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6.65	HSO4-	B (OR) 4-	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000
	HSO4-	B3O3 (OH) 4-	6.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-200	HSO4-	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000	0.00000
2	HSO4 ~	Br-	0.00000	0.00000	0.00000	0,00000,0 0,00000,0	0,0000000000000000000000000000000000000	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000
120	HSO4 - HSO4 -	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	0.00000
(23) • • • •	HSO4-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
01	HSO4-	Np02 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
222.	H504-	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
12.	HS04-	Np02 (C03) 2=-	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000
4. S.	HSO4-,	Np02 (C03)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000
1) 1))	HS04- HS04-	H2PO4- HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
11	HSO4-	P04=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-133	OH-	HC03-	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000
in :	OH-	C03*	-0.01700	~0.01000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
- 10	OH-	B(OH)4-	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000.0 0.00000	0.00000	0.00000.0 00000.0	0.00000	0.00000	0.00000
tent Eres	он- он-	B303 (OH) 4- B405 (OH) 4=	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2.43	OH-	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
÷≜¢	OH-	Am (CO3)2-	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	OK-	Am(CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1,65	OH-	C104~	0.00000 0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
्रद्धः १४३	OH- OH-	NpO2 (OH) 2- NpO2CO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
÷ 14,	OH-	Np02(C03)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-080	OH-	Np02 (C03) 3 *=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5.5	OH-	H2P04-	0.00000	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
253 253	OH-	HPO4≈	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000	0.00000 0.00000	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000
(* 3 (* 4	OH-	PO4=~ CO3=	0.00000	0.01200	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
205	HCO3 ~ HCO3 ~	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
306	нсоз-	B3O3 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
66°	HCO3~	B405 (OH) 4≈	0.0000	0.00000	0.00000	0.00000	D.00000	0.00000	0.00000	0.00000	0.00000	0.00000
642	HC03~	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
679	HC03-	Am(CO3)2~	0.00000	0.00000 0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000 0.00000
0.0 201	нсоз~ нсоз~	Am(CO3)3=- C1O4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
002	HCO3 -	NpO2 (0H) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
402	HC03~	Np02c03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	HCO3~	Np02 (C03) 2=-	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5A5	HCO3-	NpO2(CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
್ ಕಲ್ಲಿ ಕರ್ಷ	HCO3- HCO3-	H2PO4- HPO4≠	0.00000	0.00000 0.00000	0.00000	0.00000	0,00000 0,00000	0.00000	0.00000	0.00000	0.00000 0.00000	0.00000
-002	HC03-	P04=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
663	CO3=	B(OH) 4 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6F.)	C03=	B303 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
(1	CO3≠	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000
677	CO3=	Br-	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
873 3	CO3= CO3=	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	0.00000
512	co3=	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2 T C	CO3=	Np02(OH)2~	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
<i>{</i> ,7	c03=	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
£75 175	CO3= CO3=	NpO2 (CO3) 2≈~	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-001	C03≠	NpO2 (CO3)3≈=- H2PO4-	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
58 ·	CO3 =	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
÷	C03 =	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	B(OH)4-	B303 (OH) 4 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
(A4 (3.5	B(OH)4- B(OH)4-	B4O5 (OH) 4= Br-	0.00000	0,00000,0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000	0.00000	0.00000
	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
127	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
6m)	B(OH)4-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	B(OR)4-	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
(3) 20-	B(OR)4- B(OR)4-	NpO2CO3 - NpO2 (CO3) 2=-	0.00000 0.00000	0,00000 0,00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000
	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
<u> </u>	B (OH) 4-	H2P04-	0.00000	0.00050	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000	0.00000
500	B(OH)4-	HPO4=	0.00000	0.00000	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	B (OH) 4-	P04 =-	0.00000	0.00050	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	B3O3 (OH) 4- B3O3 (OH) 4-	B4O5 (OH) 4= Br-	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000
	B303 (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 0.00000	0.00000
303	B303 (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
τh.,	B3O3 (OH) 4-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000.0
7	B303 (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
751- 7526	B3O3 (OH) 4- B3O3 (OH) 4-	NpO2CO3+	0.00000	0.00000 0.000no	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
203	B303 (OH) 4- B303 (OH) 4-	NpO2 (CO3) 2=- NpO2 (CO3) 3=*-	0.00000	0,00000 0,00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0,00000.0	0.00000
	B303 (OR) 4-	H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
÷., č	B303 (OH) 4-	HP04=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.17	B303 (OH) 4~	P04=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
109 704	B405 (OH) 4= B405 (OH) 4=	Br- Am (CO3) 2	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	B405 (OH) 4= B405 (OH) 4=	Am (CO3) 2=+	0.00000	0.00000	0.00000	0.00000.0	0.00000	0.00000 0.00000	0.00000 0.00000	0,00000	0.00000	0.00000
2	B405 (OH) 4=	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000
$\mathcal{T} : \mathcal{T}$	B405 (OH) 4=	NpG2(OH)2+	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

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:• • •	B405 (OH) 4=	Np02003-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
: · :	B405 (OH) 4=	Np02 (C03) 2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000010	0.00000	0.00000
7.5	B405 (OH) 4 ≭	Np02 (C03) 3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000.0	0.00000	0.00000
210	B4O5 (OH) 4≠	H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
? : ;	B405 (OH) 4=	HPO4=	0.00000	0.00000.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
271 773	B405 (OH) 4=	PO4=- Am(CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000
	Br- Br-	Am(CO3)3*-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
- 12. 70 -	Br-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000
702	Br-	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
202	Br-	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
×2.	Br-	Np02 (C03) 2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.0	Br-	Np02(C03)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7.45	Br-	H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000	0.00000	0.00000	0.0000.0	0.00000	0.00000
 	Br-	HPO4= PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000
7	Br- 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
2.5	Am (CO3) 2-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7.1	Am (CO3) 2-	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	D.00000	0.00000	0.00000	0.00000
÷	Am (CO3) 2 -	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
70%	Am (CO3) 2-	Np02(C03)2≈-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
20/	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
70.	Am (CO3)2- Am (CO3)2-	H2P04- HP04=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000 0.00000
2.7	Am (CO3) 2-	PQ4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	Am (CO3)3≠-	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
709	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
2	Am (CO3)3=-	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
24	Am (CO3)3=-	Np02 (C03) 2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
743 743	Am (CO3)3=-	NpO2 (CO3) 3==- H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000
	Am (CO3)3=- Am (CO3)3=-	H2P04- HP04=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
145	Am (CO3) 3=-	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000
2.40	C104-	Np02 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
277	C104-	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
700	C104-	NpO2(CO3)2≈-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000.0	0.00000	0.00000
74.3	C104-	NpO2 (CO3) 3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
- 102	C104-	H2P04- HP04=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000 0.00000
201 762	C104- C104-	P04=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000
71.2	NpO2 (OH) 2-	Np02C03 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
?fu	NpO2 (OH) 2-	Np02(C03)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000.0	0.00000	0.00000
255	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
-55	NpOZ (OH) 2-	H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000.0	0.00000	0.00000
757	NpO2 (OH) 2-	HPO4=	0.00000	0.00000.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000.0	0.00000	0.00000
783 758	NpO2 (OH) 2-	PO4=- NpO2(CO3)2≈-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000
76.1	Np02C03- Np02C03-	Np02 (C03) 3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000
78.	Np02C03-	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
244	Np02C03-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
763	Np02C03-	FO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
204	NpO2 {CO3 } 2=-	Np02 (CO3) 3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
265 244	NpO2 (CO3) 2=-	H2F04- HP04=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.000000	0.00000	0.00000 0.00000
5.	NpO2(CO3)2=- NpO2(CO3)2=-	P04=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
335	NpO2 (CO3) 3==-	H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7.35	Np02(C03)3==-	HP04=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
225	NpO2(CO3)3==-	PO4 = -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
77:	H2P04-	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
772 773	H2PO4- HPO4=	P04=- P04=-	0.00000	0.00000	0.00000	0.00000	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
774	AFO44	FQ4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
· 774,			Th++++	U02++	NpO2+							
	Ċ1-	SO4=	0.00000	0.00000	0.00000							
	C1-	HS04 -	0.00000	0.00000	0.00000							
778 		OH-	0.00000	0.00000	0.00000							
	Cl- Cl-	HCO3- CO3=	0.00000	0.00000	0.00000							1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 -
70	c1-	B(OH)4+	0.00000	0.00000	0.00000							£
	ç1-	B303 (OH) 4-	0.00000	0.00000	0.00000						ŀ	
	C1-	B405 (OH) 4=	0.00000	0.00000	0.00000						£.	r. ¹
	¢1-	Br-	0.00000	0.00000	0.00000							Š
	C1-	Am (CO3) 2-	0.00000	0.00000	0.00000						· · /	
- 763 763	Cl- Cl-	Am(CO3)3=- ClO4-	0.00000	0.00000	0.00000						×,	
	C1-	Np02 (OH) 2-	0.00000	0.00000	0.00000							1 41
	ç1-	Np02C03-	0.00000	0.00000	0.00000							
7	C1-	Np02 (C03) 2=-	0.00000	0.0000	0.00000							
7t	C1-	Np02 (C03) 3==-	0.00000	0.00000	0.00000							
	C1- C1-	H2P04 -	0.00000	0.00000	0.00000							
- 83 704		HPO4= PO4=-	0.00000	0.00000	0.00000							
705	S04=	HS04-	0.00000	0.00000	0.00000							
704	S04=	OH-	0.00000	0.00000	0.00000							
3-4	S04=	HCO3-	0.00000	0.00000	0.00000							
795		C03=	0.00000	0.00000	0.00000							
799	SO4≖ SO4≖	B(OH)4-	0.00000	0.00000	0.00000							
		B303 (OH) 4-		0.00000	0.00000							
800 80 i	SO4=	B405(OH)4=										
30+	SO4= SO4=	B405 (OH) 4= Br-	0.00000	0.00000	0.00000							



823					
	504=	Am (CO3) 2-	0.00000	0.00000	0.00000
Cont	504=	Am (CO3) 3=-	0.00000	0.00000	0.00000
805	SO4=	C104-	0.00000	0.00000	0.00000
800	504=	Np02 (OH) 2-	0.00000	0.00000	0.00000
307	S04=		0.00000	0.00000	0.00000
- 502 502	S04=	Np02C03-	0.00000	0.00000	0.00000
		Np02(C03)2=-	0.00000	0.00000	0.00000
- 609		Np02(C03)3==-			
- 615		H2P04-	0.00000	0.00000	0.00000
5.1	504=	HPO4 =	0.00000	0.00000	0.00000
512	504=	PO4=-	0.00000	0.00000	0.00000
312	HSO4-	OH-	0.00000	0.00000	0.00000
814	HS04-	нсоз-	0.00000	0.00000	0.00000
ê16	HS04-	CO3=	0.00000	0.00000	0.00000
<15	HSO4-	B (OH) 4 -	0.00000	0.00000	0.00000
< ?	HS04-	B303 (OH) 4-	0.00000	0.00000	0.00000
8.13	HS04-	B405 (OH) 4 =	0.00000	0.00000	0.00000
5.0	HS04-	Br-	0.00000	0.00000	0.00000
1.1	HSO4 -	Am (CO3) 2 -	0.00000	0.00000	0.00000
8.2.1	HSO4-	Am (CQ3)3=-	0.00000	0.00000	0.00000
22L	HS04-	C104-	0.00000	0.00000	0.00000
<i>2</i> ```S	HS04-	Np02 (OH) 2-	0.00000	0.00000	0.00000
201	HS04-	Np02C03-	0.00000	0.00000	0.00000
	HSO4	Np02(CQ3)2=-	0.00000	0.00000	0.00000
÷ .	HS04-	Np02 (C03)3==-	0.00000	0.00000	0.00000
	HS04-	H2P04-	0.00000	0.00000	0.00000
et 29	HSO4~	HPO4 =	0.00000	0.00000	0.00000
<229	HSO4 -	PO4=-	0.00000	0.00000	0.00000
283	OH-	HC03 ~	0.00000	0.00000	0.00000
33	OH-	CO3=	0.00000	0.00000	0.00000
- 252	OH-	B(OH)4-	0.00000	0.00000	0.00000
8 N.)	OH-	B3O3 (OH) 4-	0.00000	0.00000	0.00000
0.54	OH-	B405 (OH) 4=	0.00000	0.00000	0.00000
ನ್ನು	OH-	Br-	0.00000	0.00000	0.0000
23.0	OH-	Am (CO3) 2 -	0.00000	0.00000	0.00000
837	OH-	Am.(CO3)3≠-	0.00000	0.00000	0.00000
939) 1939	OH-	C104~	0.00000	0.00000	0.00000
÷.)	OH-	Np02 (OH) 2 -	0.00000	0.00000	0,00000
· · · · · ·	OH-	Np02C03-	0.00000	0.00000	0.00000
2.41	OH-	Np02 (CO3) 2=-	0.00000	0.00000	0.00000
842	OH-	NpO2 (CO3) 3==-	0.00000	0.0000	0.00000
310	OH-	H2P04 -	0.00000	0.00000	0.00000
14	OH-	HPO4≈	0.00000	0.00000	0.00000
÷~ :	OH-	PO4=~	0.00000	0.00000	0.00000
()	нсоз~	C03#	0.00000	0.00000	0.00000
₹.÷	HCO3~	B(OH)4-	0.00000	0.00000	0.00000
542	HCO3~	B303 (OH) 4-	0.00000	0.0000	0.00000
94	HCO3~	B405 (OH) 4=	0.00000	0.00000	0.00000
1994 - V		Br-	0.00000	0.00000	0.00000
21	нсоз~	Am (CQ3)2-	0.00000	0.00000	0.00000
ê.	HCO3 ~	Am (CQ3)3=-	0.00000	0.00000	0.00000
803 364	HCO3~	C104~	0.00000	0.00000	0.00000
10	HCO3 ~	Np02 (OH) 2-	0.00000		0.00000
100 1000	HCO3~ HCO3~	Np02C03- Np02(C03)2=-	0.00000	0.00000	0.00000
â	HCO3~	Np02 (C03) 3==-	0.00000	0.00000	
255		mbos (602) 26	0.00000		
		H2PO4-	0.00000		0.00000
	нсоз~	H2PO4 - HPO4≈	0.00000	0.00000	0.00000
605	нсоз ~ нсоз ~	HPO4≈	0.00000	0.00000	
259 807	нсоз ~ нсоз ~ нсоз ~	HPO4≈ PO4≈~	0.00000 0.00000	0.00000 0.00000 0.00000	0.00000
259 802 804	нсо3 ~ нсо3 ~ нсо3 ~ со3 =	HPO4≈ PO4≠~ B(OH)4-	0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000
259 807 851 851 853	HCO3~ HCO3~ HCO3~ CO3= CO3*	HPO4≈ PO4≈~ 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 0.00000 0.00000 0.00000 0.00000
209 807 804 804 804 804 804	HCO3~ HCO3~ HCO3~ CO3= CO3* CO3=	HPO4≈ PO4≈~ B (OH) 4- 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 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
209 202 202 202 202 202 202 202 202 202	HC03~ HC03~ C03= C03= C03= C03=	HPO4≈ PO4≈~ B(OH)4- B3O3(OH)4- B4O5(OH)4= Br-	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
200 200 200 200 200 200 200 200 200 200	HCO3 ~ HCO3 ~ HCO3 ~ CO3 = CO3 = CO3 = CO3 = CO3 =	HPO4≈ PO4≈~ B(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2-	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HC03~ HC03~ C03= C03= C03= C03=	HPO4≈ PO4≈~ B(OH)4- B3O3(OH)4- B4O5(OH)4= Br-	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3- HCO3- CO3- CO3= CO3= CO3= CO3= CO3= CO3=	HPO4≈ PO4≈- B(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- ClO4~	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3 ~ HCO3 ~ HCO3 ~ CO3 = CO3 = CO3 = CO3 = CO3 = CO3 = CO3 = CO3 = CO3 =	HPO4≈ PO4≈- B(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- C1O4- MpO2(OH)2-	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3- HCO3- HCO3- CO3= CO3= CO3= CO3= CO3= CO3= CO3= CO3=	HPO4≈ PO4=- B(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OH)2- NpO2CO3-	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3 - HCO3 - CO3 = CO3 =	HPO4≈ PO4≈ B(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- C104~ NpO2(OH)2- NpO2(OH)2- NpO2(CO3)2=-	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3 - HCO3 - HCO3 - CO3 = CO3 =	HPO4≈ PO4≈- B(OH)4- B3O3(OH)4- B3O3(OH)4- B3O3(OH)4- B3O3(OH)4- B3C- Am(CO3)2- Am(CO3)2- Am(CO3)2- NpO2(CO3)2- NpO2(CO3)2=- NpO2(CO3)2=-	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3- HCO3- HCO3- CO3= CO3= CO3= CO3= CO3= CO3= CO3= CO3=	HPO4≈ PO4≈- B(OH)4- B303(OH)4- B405(OH)4= Br- Am(CO3)2- Am(CO3)3=- Cl04- NpO2(OH)2- NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=-	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3- HCO3- CO3= CO3= CO3= CO3= CO3= CO3= CO3= CO3=	HPO4≈ PO4≈ B(OH)4- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2- Am(CO3)3=- ClO4- NpO2(OH)2- NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)3==- H2PO4- H2PO4=	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ B(OH)4- B3O3(OH)4- B3O3(OH)4- B3O3(OH)4- B3O3(OH)4- Am(CO3)2- Am(CO3)2- NpO2(OH)2- NpO2(OH)2- NpO2(OG)2- NpO2(CO3)2=- NpO2(CO3)2=- HPO4= HPO4≈ PO4=-	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3 ~ HCO3 ~ HCO3 - CO3 = CO3	HPO4≈ PO4≈- B(OH) 4- B303(OH) 4- B405(OH) 4= Br- Am(CO3) 2- Am(CO3) 3=- C104~ NpO2(CO3) 3=- NpO2(CO3) 2=- NpO2(CO3) 2=- H2PO4= HPO4≈ PO4=- B303(OH) 4-	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.00000 0.000000 0.0000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.00000000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ B(OH)4- B3O3(OH)4- B3O3(OH)4- B3O3(OH)4- B3O3(OH)4- Am(CO3)2- Am(CO3)2- NpO2(OH)2- NpO2(OH)2- NpO2(OG)2- NpO2(CO3)2=- NpO2(CO3)2=- HPO4= HPO4≈ PO4=-	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈- B(OH) 4- B3O3(OH) 4- B3O3(OH) 4- B3O3(OH) 4- B3O3(OH) 4- B3O3(OH) 2- NpO2(O3) 2- NpO2(O3) 2- NpO2(O3) 2- NpO2(C03) 2=- NpO2(C03) 2=- NpO2(C03) 2=- HPO4- HPO4- B3O3(OH) 4- B4O5(OH) 4= B3r-	0.0000 0.0000	0.0000 0.0000	0.00000 0.000000 0.000000 0.000000 0.00000000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈- B(OH) 4- B3O3(OH) 4- B4O5(OH) 4= Br- Am(CO3)2- Am(CO3)2- Am(CO3)3=- C104~ NpO2(OH)2- NpO2(CO3)2=- NpO2(CO3)2=- HPO4≈ PO4=- B3O3(OH)4- B4O5(OH)4= Br- Am(CO3)2-	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.00000 0.000000 0.000000 0.000000 0.000000 0.00000000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈- B(OH) 4- B3O3(OH) 4- B3O3(OH) 4- B3O3(OH) 4- B3O3(OH) 4- B3O3(OH) 2- NpO2(O3) 2- NpO2(O3) 2- NpO2(O3) 2- NpO2(C03) 2=- NpO2(C03) 2=- NpO2(C03) 2=- HPO4- HPO4- B3O3(OH) 4- B4O5(OH) 4= B3r-	0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.0000	0.00000 0.00000
2000-00-00-00-00-00-00-00-00-00-00-00-00	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ B(OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am (CO3) 2- Am (CO3) 2- Am (CO3) 2- NpO2 (CO3) 2=- NpO2 (CO3) 2=- NpO2 (CO3) 2=- HPO4≈ B303 (OH) 4- B303 (OH) 4= Br- Am (CO3) 2- Am (CO3) 3=-	0.0000 0.00000 0.000000	0.0000 0.0000	0.00000 0.000000 0.000000 0.000000 0.00000000
2007-00-00-00-00-00-00-00-00-00-00-00-00-	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ B(OH) 4- B303 (OH) 4- B405 (OH) 4= BT- Am(CO3) 2- Am(CO3) 2- Am(CO3) 2- NpO2 (OH) 2- NpO2 (OG) 2- NpO2 (CO3) 2=- HPO4= HPO4= HPO4= B303 (OH) 4- B405 (OH) 4= BT- Am(CO3) 2- Am(CO3) 2- Am(CO3) 3=- CLO4-	0.0000 0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.000000 0.000000 0.000000 0.00000000	0.0000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000 0.00000 0.000000 0.00000000	0.00000 0.000000 0.00000 0.00000000
	HCO3 ~ HCO3 ~ HCO3 ~ CO3 = CO3	HPO4≈ PO4≈ B(OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 3=- C104~ NpO2 (OH) 2- NpO2 (CO3) 3=- HPO4= PO4=- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3)	0.0000 0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.0000000 0.00000000	0.00000 0.000000 0.000000 0.000000 0.00000000	0.00000 0.00000000
2007-00-00-00-00-00-00-00-00-00-00-00-00-	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ B(OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 3=- Cl04- NpO2 (CO3) 2=- NpO2 (CO3) 2=- NpO2 (CO3) 2=- HPO4= PO4= B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 2=- Cl04- NpO2(OH) 2- NpO2(OH) 2- NpO2(OH) 2- NpO2(OH) 2- NpO2(OH) 2- NpO2(OH) 2- NpO2(OH) 2- NpO2(OH) 2-	0.0000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	0.0000 0.0000	0.00000 0.000000 0.000000 0.000000 0.000000 0.00000000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HP04≈ P04≈ B(OH) 4- B303 (OH) 4- B303 (OH) 4- B303 (OH) 4- B303 (OH) 4- B303 (OH) 4- Mp02 (C03) 2- Mp02 (C03) 2- Np02 (C03) 2- Np02 (C03) 2- HP04≈ HP04≈ HP04≈ HP04≈ B303 (OH) 4- B303 (OH) 4- B3r- Am(C03) 2- Am(C03) 2- C104- Np02 (C03) 2- Np02 (C03) 2-	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000	0.0000 0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.000000 0.00000000	0.00000 0.000000 0.000000 0.00000000
2001130445001500017120045055000145084550	HCO3 - HCO3 - HCO3 - CO3 = CO3	HP04≈ P04≈ B(OH) 4- B303 (OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am (CO3) 2- Am (CO3) 2- Np02 (O3) 2- Np02 (O3) 2=- Np02 (CO3) 2=- HP04≈ HP04≈ B303 (OH) 4- B405 (OH) 4= Br- Am (CO3) 2- Am (CO3) 2- Am (CO3) 2- Cl04- Np02 (CO3) 2=- Np02 (CO3) 2=- Np03 (CO3) 2=- Np0	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000		0.00000 0.000000 0.00000000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ PO4≈- B(OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 2- Am(CO3) 2- NpO2 (CO3) 2- NpO2 (CO3) 2=- HPO4= PO4=- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 2- NpO2 (OG3) 2=- NpO2 (CO3) 2=-	0.0000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000000		0.00000 0.000000 0.000000 0.000000 0.00000000
	HCO3- HCO3- HCO3- HCO3- CO3= CO3= CO3= CO3= CO3= CO3= CO3= CO3=	HPO4≈ PO4≈ B(OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 3=- Cl04- NpO2 (CO3) 2=- NpO2 (CO3) 3=- H2PO4- HPO4= PO4=- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 2- Am(CO3) 3=- Cl04- NpO2 (CO3) 3=- Cl04- NpO2 (CO3) 3=- H2PO4- HPO4= NpO2 (CO3) 3=- H2PO4= HPO4= HPO4= HPO4= PO4=- HPO4= HPO4= PO4=- HPO4= HP	0.0000 0.00000 0.0000000 0.000000 0.000000 0.00000000		0.00000 0.000000 0.000000 0.000000 0.00000000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ PO4≈- B(OH) 4- B303 (OH) 4- B405 (OH) 4= BT- Am (CO3) 2- Am (CO3) 2- NpO2 (OB) 2- NpO2 (OG) 2- NpO2 (OG) 2- NpO2 (CO3) 2=- HPO4= B303 (OH) 4- B405 (OH) 4= BT- Am (CO3) 2- Am (CO3) 2- Am (CO3) 2- Am (CO3) 2- NpO2 (CO3) 2=- NpO2 (CO3) 2=- NpO3 (CO3) 2=-	0.0000 0.00000 0.0000 0.000000 0.000000 0.000000 0.00000000		0.00000 0.000000 0.000000 0.000000 0.00000000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ PO4≈- B(OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 2- Am(CO3) 2- NpO2 (OH) 2- NpO2 (CO3) 2=- NpO2 (CO3) 2=- HPO4≈ PO4≈- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2=- NpO2 (OG3) 2=- NpO2 (CO3) 2=- NpO3 (CO3) 2=- NpO4=- B405 (OH) 4= Br-	0.0000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000		0.00000 0.000000 0.000000 0.00000000
	HC03- HC03- HC03- CO3= CO3= CO3= CO3= CO3= CO3= CO3= CO3=	HPO4≈ PO4≈ PO4≈- B(OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 3=- C104- NpO2 (CO3) 3=- HPO4- NpO2 (CO3) 3=- HPO4= PO4=- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- NpO2 (CO3) 3=- HPO4= NpO2 (CO3) 3=- HPO4= PO2=- NpO2 (CO3) 3=- HPO4= PO4=- PO2=- NpO2 (CO3) 3=- HPO4= PO4=- PO4=- PO2=- NpO2 (CO3) 3=- HPO4=- PO4=- PO4=- PO4=- PO4=- PO4=- HPO4=- PO4=- PO4=- HPO4=- PO4=- PO4=- HPO4=- PO4=- PO4=- HPO4=- PO4=- PO4=- HPO4=- PO4=- HPO4=- PO4=- PO4=- HPO4=- PO4=- HPO4=- PO4=- HPO4=- HPO4=- PO4=- H	0.0000 0.00000 0.000000 0.000000 0.000000 0.00000000		0.00000 0.000000 0.00000000
	HCO3 - HCO3 - HCO3 - CO3 = CO3	HPO4≈ PO4≈ PO4≈- B(OH) 4- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2- Am(CO3) 2- Am(CO3) 2- NpO2 (OH) 2- NpO2 (CO3) 2=- NpO2 (CO3) 2=- HPO4≈ PO4≈- B303 (OH) 4- B405 (OH) 4= Br- Am(CO3) 2=- NpO2 (OG3) 2=- NpO2 (CO3) 2=- NpO4=- B405 (OH) 4= Br-	0.0000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000		0.00000 0.000000 0.000000 0.00000000



Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

643					P_AM.CH		
	B303 (OH) 4-	Np02 (OH) 2-	0.00000	0.00000	0.00000		
64		Np02C03-	0.00000	0.00000	0.00000		
295		Np02 (C03) 2=~	0.00000	0.00000	0.00000		
	\$303 (OH) 4-	Np02 (C03) 3==-					
37.1		H2P04-	0.00000	0.00000	0.00000		
	B3O3 (OH) 4-	HPO4=	0.00000	0.00000	0.00000		
	B3O3 (OH) 4-	PO4=-	0.00000		0.00000		
	B405 (OH) 4=	Br-	0.00000	0.00000	0.00000		
	B405 (QH) 4=	Am (CO3) 2-	0.00000		0.00000		
	B405 (OH) 4=	Am (CO3) 3=-	0.00000		0.00000		
	B405 (OH) 4=	C104-	0.00000	0.00000	0.00000		
	B405 (OH) 4=	NpQ2 (OH) 2-	0.00000		0.00000		
	8405 (OH) 4=	Np02C03-	0.00000		0.00000		
	B4Q5 (OH) 4=	Np02(C03)2*-	0.00000	0.00000	0.00000		
	B405 (OH) 4=	Np02 (C03) 3==-		0.00000	0.00000		
	B405 (OH) 4≈	H2P04-	0.00000	0.00000	0.00000		
	B405 (OH) 4=	HPO4=	0.00000	0.00000	0.00000		
	B405 (OH) 4=	P04=-	0.00000	0.00000	0.00000		
. • •	Br-	Am (CO3) 2 -	0.00000	0.00000	0.00000		
81 C -	Br-	Am (CO3)3=-	0.00000	0.00000	0.00000		
2.3	Br-	C104-	0.00000		0.00000		
91X	Br-	Np02 (OH) 2-	0.00000	0.00000	0.00000		
	Br-	Np02C03-	0.00000	0.00000	0.00000		
	Br-	Np02 (C03) 2=-	0,00000	0.00000	0.00000		
	Br-	Np02(C03)3==-		0.00000	D.00000		
: î :-	Br-	H2PO4-	0.00000	0.00000	0.00000		
	Br-	HPO4=	0.00000	0.00000	0.00000		
		PO4 = -	0.00000	0.00000	0.00000		
		Am (CO3)3=-	0.00000	0.00000	0.00000		
	Am (CO3) 2 -	C104-	0.00000	0.00000	0.00000		
	Am (CO3) 2-	Np02 (OH) 2-	0.00000	0.00000	0.00000		
		Np02C03-	0.00000	0.00000	0.00000		
200	Am (CO3)2-	Np02(C03)2=-		0.00000	0.00000		
	Am (CO3) 2-	NpO2 (CO3) 3≠≈-		0.00000	0.00000		
27	Am (CO3) 2-	H2P04~	0.00000	0.00000	0.00000		
		HP04=	0.00000	0.00000	0.00000		
	Am (CO3) 2-	PO4 = -	0.00000	0.00000	0.00000		
	Am (CO3)3=-	C104-	0.00000	0.00000	0.00000		
		Np02 (OH) 2-	0.00000	0.00000	0.00000		
	Am(CO3)3=-	Np02C03-	0.00000	0.00000	0.00000		
	Am(CO3)3=-	Np02 (C03) 2=-		0.00000	0.00000		
	Am(CO3)3=-	Np02 (C03) 3=-		0.0000	0.00000		
	Am (CO3) 3=-	H2P04-	0.00000	0.00000	0.00000		
	Am(CO3)3=-	HPO4=	0.00000	0.00000	0.00000		
		PO4=-	0.00000	0.00000	0.00000		
	C104- C104-	Np02 (OH) 2- Np02C03-	0.00000	0.00000	0.00000		
	C104-	Np02(C03)2=-	0.00000	0.00000	0.00000		
	C104-	Np02 (C03) 3==-		0.00000	0.00000		
	C104-	H2P04-	0.00000	0.00000	0.00000		
		HPO4=	0.00000	0.00000	0.00000		
		P04=-	0.00000	0.00000	0.00000		
	NpO2 (OH) 2-	Np02C03-	0.00000	0.00000	0.00000		
	Np02(0H)2-	ND02 (C03) 2=-		0.00000	0.00000		
		Np02 (C03) 3==-		0.00000	0.00000		
	NpO2 (OH) 2-	H2P04-	0.00000	0.00000	0.00000		
		HPO4=	0.00000	0.00000	0.00000		
	NpO2 (OH) 2-	P04=-	0.00000	0.00000	0.00000		
	NpO2C03-	Np02 (CO3) 2=-	0.00000	0.00000	0.00000		
	NpO2CO3 -	Np02 (C03) 3==-		0.00000	0.00000		
	Np02C03-	HZPO4-	0.00000	0.00000	0.00000		
	Np02C03-	HPO4=	0.00000	0.00000	0.00000		
55	Np02C03-	P04=-	0.00000	0.00000	0.00000		
	NpO2 (CO3) 2=-	Np02 (CO3) 3=*-	0.00000	0.00000	0.00000		
57	NpO2 (CO3) 2=-	H2P04-	0.00000	0.00000	0.00000		
<u>'S</u> ?	NpO2 (CO3) 2=-	HP04=	0.00000	0.00000	0.00000		
41	NpO2 (CO3)2=-	P04=-	0.00000	0.00000	0.00000		
5	NpO2 (CO3)3==-	H2P04-	0.00000	0.00000	0.00000		
	NpO2 (CO3) 3==-	HPO4=	0.00000	0.00000	0.00000		
			0.00000	0.00000	0.00000		
1.2	NpO2 (CO3) 3==-	PO4=-		0 00000			
102 103	NpO2 (CO3) 3==- H2PO4-	PO4=- HPO4=	0.00000	0.00000	0.00000		
102 103 451	NpO2 (CO3)3==- H2PO4- H2PO4-		0.00000	0.00000	0.00000		
622 103 441 455	NpO2 (CO3) 3==- H2PO4-	HPO4=					
102 103 イン 大手	NpO2 (CO3) 3==- H2PO4- H2PO4- HPO4=	HP04= P04=- P04=-	0.00000 0.00000	0.00000 0.00000	0.00000		
102 103 イント やい 107	NpO2 (CO3)3==- H2PO4- H2PO4-	HP04= P04=- P04=-	0.00000 0.00000	0.00000	0.00000		
102 103 145 145 145 145 145 145 145 145 145 145	NpO2 (CO3) 3==- H2PO4- H2PO4- HPO4=	HPO4= PO4=- PO4=- Binary Intera	0.00000 0.00000 ctions: la	0.00000 0.00000 mbda(n,c)	0.00000 0.00000 .		
22 20 20 20 20 20 20 20 20 20 20 20 20 2	NDO2(CO3)3==- H2PO4- K2PO4- HPO4= Neutral-Cation	HP04= P04=- P04=- Binary Intera C02(aq)	0.00000 0.00000 ctions: la CaCO3(ag)	0.00000 0.00000 mbda(n,c) MgCC3(aq)	0.00000 0.00000 . B(OH)3(ag)	NpO2OH (aq)	
	NpO2 (CO3)3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+	HP04= P04=- P04=- Binary Intera C02(aq) 0.10000	0.00000 0.00000 ctions: la CaCO3(aq) 0.00000	0.00000 0.000000 mbda(n,c) MgCC3(aq) 0.00000	0,00000 0,00000 . B(OH)3 (ag) -0,09700	0.0000	0.00000
	NpO2 (CO3) 3==- H2PO4- K2PO4- HPO4= Neutral-Cation Na+ K+	HP04= P04=- P04=- Binary Intera C02(aq) 0.10000 0.05100	0.00000 0.00000 ctions: la CaCO3(aq) 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000	0.00000 0.00000 . B(OH)3(ag) -0.09700 -0.14000	0.00000	0.00000
	NpO2 (CO3)3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++	HP04= P04=- P04=- Binary Intera C02(aq) 0.10000 0.05100 0.18300	0.00000 0.00000 ctions: la CaCO3(ag) 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000	0.00000 0.00000 . B(OH)3(aq) -0.09700 -0.14000 0.00000	0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000
	NpO2 (CO3)3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++ Mg++	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.05100 0.18300 0.18300	0.00000 0.00000 ctions: la 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 B(OH)3(aq) -0.09700 -0.14000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000
	NpO2(CO3)3==- H2PO4- H2PO4- HPO4= HPO4= Neutral-Cation Na+ K+ Ca++ Mg++ MgOH+	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.05100 0.18300 0.18300 0.00000	0.00000 0.00000 ctions: la CaCO3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 -0.09700 -0.14000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000 0.00000
	NpO2(CO3)3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++ MgOH+ H+	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.05100 0.18300 0.18300 0.18300 0.00000 0.00000	0.00000 0.00000 ctions: la CaCO3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n.c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 -0.09700 -0.14000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000 0.00000 0.00000 0.29000
	NpO2 (CO3)3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++ MgO++ H4 MgB(OH)4+	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.18300 0.18300 0.18300 0.00000 0.00000 0.00000	0.00000 0.00000 ctions: la CaCO3(ag) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 -0.09700 -0.14000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000 0.00000 0.29000 0.29000 0.00000
	NpO2 (CO3) 3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++ Mg++ Mg0H+ H4- MgB (OH) 4+ CaB (OH) 4+	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.05100 0.18300 0.18300 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 ctions: la CaCO3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	C.00000 0.00000 -0.09700 -0.14000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000 0.00000 0.29000 0.00000 0.00000
	NpO2 (CO3)3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++ MgOH+ H+ MgC(OH)4+ CaB(OH)4+ Am+++	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.05100 0.18300 0.18300 0.18300 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 ctions: la CaCO3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 -0.09700 -0.14000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000 0.00000 0.29000 0.00000 0.00000 0.00000
902 909 909 909 909 909 909 909 909 909	NpO2 (CO3) 3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++ Mg++ Mg++ H+ MgB (OH) 4+ CaB (OH) 4+ Am+++ Am+++ Am+++	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.18300 0.18300 0.18300 0.00000 0.00000 0.00000 0.00000 0.00000	6.60000 0.00000 ctions: la CaCO3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	C.00000 0.00000 -0.09700 -0.09700 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000 0.00000 0.29000 0.00000 0.00000 0.00000
2022 2023 2024 2025 2025 2025 2025 2025 2025 2025	NpO2 (CO3) 3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++ Mg++ Mg0H+ H+ MgE (OH) 4+ CaB (OH) 4+ AmcO3+ Th++++	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.05100 0.18300 0.18300 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 ctions: la CaCO3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	C.00000 0.00000 -0.09700 -0.14000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000 0.29000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
2022 2023 2024 2025 2025 2025 2025 2025 2025 2025	NpO2 (CO3) 3==- H2PO4- H2PO4- HPO4= Neutral-Cation Na+ K+ Ca++ Mg++ Mg++ H+ MgB (OH) 4+ CaB (OH) 4+ Am+++ Am+++ Am+++	HP04= P04=- P04=- Binary Intera CO2(aq) 0.10000 0.18300 0.18300 0.18300 0.00000 0.00000 0.00000 0.00000 0.00000	6.60000 0.00000 ctions: la CaCO3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 mbda(n,c) MgCC3(aq) 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	C.00000 0.00000 -0.09700 -0.09700 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 -0.07000 0.00000 0.00000 0.00000 0.29000 0.00000 0.00000 0.00000



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Neutral- Anior	Binary Intera	ctions: la	mbda(n,a)			
	CO2 (aq)	CaC03 (ag)	MgCO3 (ag)	B(OH)3(ag)	Np020H(aq)	H3PO4 (ag)
c1-	-0.00500	0.00000	0.00000	0.09100	0.00000	0.00000
504=	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
C03=	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
B303 (OH) 4- B405 (OH) 4=	0.0000C 0.0000C	0.00000	0.00000	0.00000	0.00000	0.00000
B405(UR)4= 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
C104-	0,00000	0.00000	0.00000	0.00000	0.00000	0.00000
Np02 (OH) 2 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Np02 (C03) 2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Np02 (C03) 3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 -0.40000
H2 PO4 - HPO4 =	0.0000C 0.0000C	0.00000	0.00000	0.00000	0.00000	0.00000
P04=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Neutral-Cation	n-Anion Termary	Interactic	ns: zeta(1	n,c,a)		
			/			
		CO2 (ag)				1p020H(ag H3P04(ag
Na+	C1-	0.00000	0.00000			0.00000 0.00000
Na+	SO4≠ HSO4∞	0.00000	0.00000			0.00000 0.00000
Na+	HSO4- OH-	0.00000	0.00000			0.00000 0.00000
Na+ Na+	HC03-	0.00000	0.00000			00000 0.00000
Na+	CO3=	0.00000	0.00000	0.00000	0.00000 0	0.00000 0.00000
Na+	B(OH)4-	0.00000	0.00000			0.00000 0.00000
Na+	B303 (OH) 4-	0.00000	0.00000			0.00000 0.00000
Na+	B405 (OH) 4≈	0.00000	0.00000			0.00000 0.00000
Na+	Br-	0.00000	0.00000			0.00000 0.00000
Na+	Am(CO3)2-	0.00000	0.00000			.00000 0.00000
Na+ Na+	Am(CO3)3=+ C1O4-	0.00000	0.00000			.00000 0.00000
Na+	NpO2 (OH) 2-	0.00000	0.00000			0.00000 0.00000
Na+	Np02C03-	0.00000	0.00000	0.00000	0.00000 0	.00000 0.00000
Na+	Np02 (C03) 2=-	0.00000	0.00000			0.00000 0.00000
Na+	NpO2(CO3)3≠=-	0.00000	0.00000			.00000 0.00000
Na+	H2PO4-	0.00000	0.00000			0.00000 0.00000
Na+	HP04 =	0.00000	0.00000			0.00000 0.00000
Na+	P04=-	0.00000	0.00000			.00000 0.00000
K+ K+	C1- S04=	0.00000	0.00000			0.00000 0.00000
K+	HS04 -	0.00000	0.00000			0.00000 0.00000
K+	OH-	0.00000	0.00000	0.00000	0.00000 0	0.0000.0 0.00000.
K+	HCO3 -	0.00000	0.00000			0.0000. 0.00000.
K+	CO3=	0.00000	0.00000			0.00000 0.00000
K+	B(OH)4-	0.00000	0.00000			0.00000 0.00000
K+	B303 (OH) 4-	0.00000	0.00000			0.00000 0.00000
K+ K+	B405 (OH) 4= Br-	0.00000	0.00000			0.00000 0.00000
K+	Am (CO3)2-	0.00000	0.00000			00000 0.00000
K+	Am (CO3)3=-	0.00000	0.00000			0.00000 0.00000
K+	C104-	0.00000	0.00000			0.00000 0.00000
K+	Np02 (OH) 2-	0.00000	0.00000	0.00000		0.00000 0.00000
K+	Np02C03-	0.00000	0.00000			0.00000 0.00000
X+	Np02 (C03) 2=-	0.00000	0.00000			0.00000 0.00000
K+ K+	Np02 (C03)3==- H2P04-	0.00000	0.00000			0.00000 0.00000
K+	HP04=	0.00000	0.00000			0.00000 0.00000
K+	PO4=-	0.00000	0.00000			0.00000 0.00000
Ca++	C1-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++	504=	0.00000	0.00000			0.00000 0.00000
Ca++	HSO4-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++	OH-	0.00000	0.00000	0.00000		0.00000 0.00000
Ça++	HC03-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++ Ca++	CO3= B(OK)4-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++	в (он) 4- взоз (он) 4-	0.00000	0.00000	0.00000		0.00000 0.000000
Ca++	B405 (OH) 4=	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++	Br-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++	Am(CO3)2-	0.00000	0.0000	0.00000		0.00000 0.00000
Ca++	Am (CO3)3=-	0.0000	0.00000	0.00000		0.00000 0.00000
Ça++	C104-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++	Np02 (OH) 2-	0.00000	0.00000	0.00000		
Ca++	Np02C03-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++ Ca++	NpO2 (CO3)2=- NpO2 (CO3)3==-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++ Ca++	H2PO4-	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++	HP04=	0.00000	0.00000	0.00000		0.00000 0.00000
Ca++	PO4 =-	0.00000	0.00000	0.00000		0.00000 0.00000

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

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5000 Mg++	C1-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1)/4 Mg++	S04=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1076 Mg++	H504-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Mg++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
(C) Mg++	HCO3-	0.00000	0.00000.0	0.00000	0.00000	0.00000	0.00000
1077 Mg++	C03=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1073 Mg++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
())) Mg++	B303 (OH) 4 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
() Mg++	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
C52 Mg++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
022 Mg++	Am (CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
`.`~ Mg++	Am (CO3)3=~	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
018 Mg++	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Mg++	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1082 Mg++	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
068 Mg++	Np02 (C03) 2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
60. Mg++	NpO2 (CO3) 3==-	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
()	H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1001 Mg++ 5021 Mg++	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
SSS MgOH+ SSSS MgOH+	C1-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgQH+	S04 = HS04 ~	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1007 MgOH+	нсоз -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	C03=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NgOH+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	B303 (OH) 4~	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	B405 (OH) 4≠	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	Am (CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	Am (CO3)3≠-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
C MgOH+	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	Np02 (C03) 2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1 EDD MgOH+	NpO2 (CO3) 3≈≉-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1112 MgOH+	H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgOH+	HPO4 =	0.00000	0.00000	0.00000	0.0000	0.00000	0.00000
MgOH+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
· () 응 H+ · · · · · · · · · · · · · · · · · · ·	C1-	0.00000	0.00000	0.00000	-0.01020	0.00000	0.00000
	SO4≈	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	HSO4 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	OK-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1917 日 + 793轮 日 +	HC03 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1110 H+	C03=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1320 H+	B (OH) 4- B3O3 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1121 H+	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
122 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
-:24 H+	Am(CO3)3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1725 H+	C104-	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
1107 H+	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1925 H+	NpO2 (CO3) 2=-	0.00000	0,00000	0.00000	0.00000	0.00000	0.00000
::::: H+	NpO2 (CO3)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1336 H+	H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
518 E H+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1102 H+	P04=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
133 MgB (QH) 4+	C1-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1 5 • MgB (OH) 4+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
135 MgB(OH)4+ 135 MgB(OH)4+	HSO4 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1331 MgB (OH) 4+ 1337 MgB (OH) 4+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgB(OH)4+	HCO3 ~ CO3 =	0.00000.0	0.00000	0.00000	0.00000	0.00000	0.00000
1233 MgB (OH) 4+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
154) MgB(OH)4+	B303 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
121 MgB (OH) 4+	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
142 MgB (OH) 4+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
42 MgB (OH) 4+	Am (CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
See MgB (OH) 4+	Am (CO3 3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1140 MgB (OH) 4+	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
11-1> MgB (OH) 4+	NpO2 (OH) 2 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgB(OH)4+	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
14名 MgB (OH) 4+	NpO2 (CO3) 2≖-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgB (OH) 4+	Np02(C03)3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
MgB(OH)4+	H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1101 MgB(OH)4+	HPO4 =	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
155. MgB(OH)4+ 155. CaB(OH)4+	P04=-	0.00000	0.00000	0.00000	0.00000	0.0000	0.00000
	C1-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	504=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
다 (OH)4+ 이 (OH)4+ 이 (OH)4+	HSO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
157 CaB(OH)4+	он- нсоз-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
155 CaB(OH)4+	CO3=	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
159 CaB(OH)4+	B(OH)4-	0.00000	0.00000	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000
	B303 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000.0	0.00000
: 1은 : CaB (OH) 4+	B405 (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



14. 3	CaB(OH)4+	Am (CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
1150	CaB(OH)4+	Am (CO3)3=+	0.00000	0.00000	0.00000	0.00000	00000.0	0.000
:::/	CaB(OH)4+	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
:::::	CaB(OH)4+	NpO2 (QH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
:17	CaB(OH)4+	Np02C03-	0,00000	0.00000	0.00000	0.00000	0.00000	0.000
÷7	CaB(OH)4+	NpO2 (CO3) 2≠-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
122	CaB (OH) 4+	NpO2 (CO3) 3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
77	CaB (OH) 4+	H2P04-	0,00000	0.00000	0.00000	0.00000	0.00000	0.000
\mathcal{V}_{i}^{\pm}	CaB(OH)4+	HPO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
71	CaB (OH) 4+	PO4=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
72	Am+++	C1-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
	Am+++	S04=	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
• *.	Am+++	HS04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
٠.	Am+++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
10	Am+++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
	Am+++	CO3=	0.00000	0.00000	0.00000	0.00000	000000.0	0.001
÷ - ;	Am+++	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
22.2		B303 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
1.1	Am+++	B405 (OH) 4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00(
1.0	Am+++	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00(
1.15	Am+++	Am (CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
: 24	Am+++	Am (CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.000
:28	Am+++	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
122	Am+++	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
117	Am+++	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
 		Np02(C03)2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
19		Np02 (C03) 3==-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
		H2P04-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
100	Am+++				0.00000	0.00000	0.00000	0:00
	Am+++	HPO4=	0.00000	0.00000 0.00000	0.00000	0.00000	00000.0	0.00
122		P04=-	0.00000			0.00000	0.00000	0.00
122	AmCO3+	C1-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
121	AmCO3+	SO4 =		0.00000	0.00000			
122	AmCO3+	H504-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
::::	AnCO.+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
7	AmCO3+	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
3.35		CO3 =	0.00000	0.00000	C.00000	0.00000	0.00000	0.00
112	AmCO3+	B (OH) 4 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
277	AmCO3+	B3O3 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	AnCO3+	B405(0H)4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
2	AmCO3+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
202	AmCO3+	Am (CO3) 2 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
2024	AmCO3+	Am (CO3)3=-	0,00000	0.00000	0.00000	0.00000	0.00000	0.00
2.25	AmCO3+	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
1.5	AmCO3+	NpO2 (OH) 2-	0.00000	0.00000.0	0.00000	00000.0	0.00000	0.00
10.02	AmCO3+	Np02003-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
:103	AmCO3+	NpO2(CO3)2=-	0,00000	0.00000	0.00000	0.00000	0.00000	0.00
200		NpO2(CO3)3**-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
.215		H2PO4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
11 fr	AmCO3+	HPO4=	g.00000	0.00000	0.00000	0.00000	0.00000	0.00
12.17	AmCO3+	PO4 = -	0,00000	0.00000	0.00000	0.00000	0.00000	0.00
:: :3		C1-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
2:4	Th++++	SO4 =	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
211	Th++++	HSO4-	0,00000	0.00000	0.00000	0.00000	0.00000	0.00
218		OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
217	Th++++	HCO3-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
215		CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
÷		B (OH) 4 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	Th++++	B303 (OH) 4-	0.00000.0	0.00000	0.00000	0.00000	0.00000	0.00
221		B405 (OH) 4=	0,00000	0.00000	0,00000	0.00000	0.00000	0.00
222		Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
222		Am (CO3) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
		Am (CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	Th++++		0.00000	0.00000	0.00000	0.00000	0.00000	0.00
		C104~	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
1220		NpO2 (OH) 2-	0,00000	0.00000	0.00000	0.00000	0.00000	0.00
222		Np02003-				0.00000	0.00000	0.00
1228	Th++++	NpO2 (CO3) 2=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	Th++++	NpO2 (CO3) 3==-	0.00000	0.00000	0.00000			0.00
1,30		HZPO4-	0.00000	0.00000		0.00000	0.00000	
12 3 I		HPO4≈	0.00000	0.0000	0.00000	0.00000	0.00000	0.00
	Th++++	PO4 = ~	0,00000	0.0000	0.00000	0.00000	0.00000	0.00
233		C1-	0.00000	0.0000	0.00000	0.00000	0.00000	0.00
	UO2++	SO4 =	0.00000	0.00000	0.00000.0	0.00000	0.00000	0.00
1206	UO2++	H504~	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
11.5%	U02++ U02++	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
	UQ2++	HCO3~	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
132	UQ2++	C03=	0,00000	0,00000	0.00000	0.00000	0.00000	0.00
233		B(OH)4-	0.00000	0.00000	0,00000	0.00000	0.00000	0.00
232		B3O3 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
239 229			0.00000	0.00000	0.00000	0.00000	0.00000	0.00
1232 1280 1280 1280	U02++	B405 (OH) 4=		0.00000	0.00000	0.00000	0.00000	0.00
1232 1280 1280 1280	U02++ U02++		0.00000		0.00000	0.00000	0.00000	0.00
1239 1290 1240 1240 1240	U02++ U02++ U02++	Br-	0.00000	0.00000	0.00000			
	UO2++ UO2++ UO2++ UO2++	Br- Am(CO3)2-	0.00000		0.00000	0.00000	0.00000	0.00
	U02++ U02++ U02++ U02++ U02++	Br- Am(CO3)2- Am(CO3)3≃-	0.00000	0.00000	0.00000	0.00000	0.00000	
1232 について いっか いっか ひろ	U02++ U02++ U02++ U02++ U02++ U02++	Br- Am(CO3)2- Am(CO3)3≃- C1O4-	0.00000 0.00000 0.00000	0.00000 0.00000	0.00000 0.00000	0.00000	0.00000 0.00000	0.00
1232 について いっか いっか いっか いっか	U02++ U02++ U02++ U02++ U02++ U02++ U02++	Br- Am(CO3)2- Am(CO3)3≈- ClO4- NpO2(OH)2-	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000	0.00000 0.00000 0.00000	0.00000 0.00000 0.00000	0.00000 0.00000 0.00000	0.00
1232 1220 1211 1240 1240 1240 1240 1240 124	U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++	Br- Am(CO3)2- Am(CO3)3=- C104- NpO2(OH)2- NpO2CO3-	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00 0.00 0.00
	U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++	Br- Am (CO3) 2- Am (CO3) 3=- C104- NpO2 (OH) 2- NpO2 (OG) 2- NpO2 (CO3) 2=-	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	0.00 0.00 0.00 0.00
	U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++	Br- Am (CO3)2- Am (CO3)3=- CLO4- NpO2(OH)2- NpO2(OH)2- 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 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00 0.00 0.00 0.00
ないではないないです。	U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++	Br- Am (CO3) 2- Am (CO3) 3= - ClO4- NpO2 (OH) 2- NpO2 (CO3) 2 NpO2 (CO3) 3==- H2PO4-	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00 0.00 0.00 0.00 0.00
12.2.2.1111はないにつける ないのかからくやけるか	U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++ U02++	Br- Am (CO3)2- Am (CO3)3=- CLO4- NpO2(OH)2- NpO2(OH)2- 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 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	00.0 00.0 00.0 00.0 00.0 00.0 00.0

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u/RT

f. f	J: OUTPUT File	6		-			
Np02+	C1-	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Np02+	SO4=	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	H5O4 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.00
Np02+	OH-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	HCO3 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	CO3=	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	B(OH)4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	B3O3 (OH) 4-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	B405 (OH) 4≠	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	Br-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	Am (CO3)2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+.	Am (CO3)3=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
NpO2+	C104-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	NpO2 (OH) 2-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	Np02C03-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	NpO2 (CO3) 2=-	0.00000 0.00000	0.00000	0.00000	0.00000	0.00000	0.0
Np02+	Np02 (C03) 3#=-	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
NpO2+	H2 P04 -	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
NpO2+	HP04 =	0.00000	0.00000	0.00000	0.00000	0.00000	0.0
NpO2+	PO4=- ZER ACTIVITY COEFFI		0.00000	0.00000			
	lance replaces elem						
this is a	BATCH problem						
Ideal Gas Temperatu	Constant is Unity	(Dimension) =] degree Ko					
115 Spe	cies	23 E	lements				
	Element Name	Molecular N	Weight				
	Hydrogen	1.00790					
	0xygen	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	28.54000					
	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					
	C104-(EL)	99.45060					
	Phosphorus	30.97400					
	Electron	0.00000					
	Charge	0.00000					
Sner	es Name		Phase	Mol.		d Chemical	Pot
		WATER	aqueous	18.0		95.663	
1 H2O		Na+	aqueous	22.9		.05.651	
1 H2O 2 Na+		K+	aqueous	39.0		.13.957	
1 H2O 2 Na+ 3 K+							
1 H2O 2 Na+ 3 K+ 4 Ca++		Ca++	aqueous	40.0	80 -2	23.300	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++		Ca++ Mg++	aqueous	40.0 24.3	80 -2 05 -1	.83.468	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH		Ca++ Mg++ MgOH+	aqueous aqueous	40.0 24.3 41.3	80 -2 05 -1 12 -2	.83.468 51.940	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH+ 7 H+		Ca++ Mg++ MgOH+ H+	aqueous aqueous	40.0 24.3 41.3 1.0	80 -2 05 +1 12 -2 08	.83.468 51.940 0.000	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH+ 7 H+ 8 C1-		Ca++ Mg++ MgOH+ H+ Cl-	aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4	80 -2 05 -1 12 -2 08 53 -	.83.468 51.940 0.000 52.955	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH+ 7 H+ 8 C1- 9 504=		Ca++ Mg++ MgOH+ H+ Cl- SO4=	aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0	80 -2 05 -1 12 -2 08 53 - 58 -3	83.468 51.940 0.000 52.955 00.386	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 Mg0H4 7 H+ 8 C1- 9 SO4= 10 HSO4-		Ca++ Mg++ MgOH+ H+ Cl- SO4= HSO4-	aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0	80 -2 05 -1 12 -2 08 53 - 58 -3 66 -3	83.468 51.940 0.000 52.955 00.386 04.942	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH+ 7 H+ 8 C1- 9 504= 10 HSO4- 11 OH-		Ca++ Mg++ MgOH+ H+ C1- SO4= HSO4- OH-	aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0	80 -2 05 -1 12 -2 08 53 - 58 -3 66 -3 07 -	.83.468 251.940 0.000 -52.955 100.386 104.942 -63.435	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 Mg0H4 7 H+ 8 C1- 9 SO4= 10 HSO4 11 OH- 12 HCO3-		Ca++ Mg++ MgOH+ C1- SO4= HSO4= OH- HCO3-	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0 61.0	80 -2 05 -1 12 -2 08 53 - 58 -3 66 -3 07 - 17 -2	83.468 51.940 0.000 52.955 100.386 104.942 -63.435 236.751	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH- 7 H+ 8 C1- 9 SO4= 10 HSO4= 11 OH- 12 HCO3- 13 CO3=		Ca++ Mg++ MgOH+ H+ C1- SO4= HSO4= OH- HCO3- CO3=	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0 61.0 60.0	80 -2 05 -1 12 -2 08 - 53 - 58 -3 66 -3 07 - 17 -2 09 -2	83.468 51.940 0.000 52.955 100.386 104.942 -63.435 236.751 212.944	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH+ 7 H+ 8 C1- 9 504= 10 HSO4- 11 OH- 12 HCO3- 13 CO3= 14 CO2 (4	.xg)	Ca++ MgOH+ H+ C1- SO4= HSO4- - OH- HCO3- CO3= CO2 (aq)	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0 61.0 61.0 60.0 44.0	80 -2 95 -1 12 -2 08 -3 53 -3 56 -3 66 -3 17 -2 09 -2 10 -1	83.468 51.940 0.000 52.955 100.386 104.942 -63.435 136.751 212.944 155.680	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 Mg0H+ 7 H+ 8 C1- 9 SO4= 10 HSO4= 10 HSO4= 11 OH- 11 CO2(11 CO2(15 CaCO)	.ug) (ag)	Ca++ Mg++ Mg0H+ H+ C1- S04= HS04- OH- HC03- C03= C02(aq) CaC03(aq)	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0 61.0 60.0 44.0 100.0	80 -2 05 -1 12 -2 08 -3 558 -3 66 -3 07 - 17 -2 09 -2 10 -1 89 -4	.83.468 :51.940 0.000 :52.955 :00.386 :04.942 :63.435 :36.751 :12.944 :55.680 :43.500	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH+ 7 H+ 8 C1- 9 SO4= 10 HS04 11 OH- 12 HCO3- 13 CO3= 14 CO2(6 15 CaCO 16 MgCO3	(aq) (aq)	Ca++ Mg++ MgOH+ 1+ C1- SO4= HSO4- . OH- HCO3- CO3= CO2(aq) MgCO3(aq)	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 61.0 60.0 44.0 100.0 84.3	80 -2 05 -1 12 -2 08 -3 558 -3 66 -3 07 - 17 -2 09 -2 10 -1 89 -4 14 -4	.83.468 :51.940 0.000 :52.955 :00.386 :04.942 :63.435 :36.751 :212.944 :55.680 :03.155	
1 H2C 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH+ 6 MgOH 7 H+ 8 C1- 9 SO4= 10 HSO4- 11 OH- 12 HCO3- 11 OH- 12 HCO3 13 CO3= 14 CO2 (d 15 CaCC) 16 MgCO 17 B (OH)	. (aq) 3 (aq) 3 (aq)	Ca++ Mg++ Hg0H+ H+ C1- SO4= - OH- HC03- C03= C02(aq) CaC03(aq) B(CH)3(aq)	àqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0 61.0 60.0 44.0 100.0 84.3 61.8	80 -2 05 -1 12 -2 08 -3 553 -3 566 -3 07 - 17 -2 09 -2 10 -1 89 -4 32 -3	.83.468 (51.940 0.000 52.955 (00.386 (04.942 -63.435 (36.751 212.944 (55.680 (43.500 (03.155) 990.810	
1 H2C 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgCH- 7 H+ 8 C1- 9 SO4= 10 HSO4- 11 OH- 12 HCO3- 13 CO3= 14 CO2(d 15 CaCC) 17 B(OH) 18 B(OH)	(ag) (ag) (ag) 3 (ag) 4 –	Ca++ Mg++ Mg0H+ H+ Cl- SO4= - OH- HC03- CO3 = CO2 (aq) B (OH) 4- B (OH) 4-	àqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8	80 -2 05 -1 12 -2 08 -3 53 -3 66 -3 07 - 17 -2 09 -2 10 -1 89 -4 32 -3 39 -4	.83.468 (51.940 0.000 52.955 (00.386 (04.942 (63.435 (36.751 112.944 (55.680 (43.500 (03.155 (90.810 (45.200	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH 7 H+ 8 CL- 9 SO4= 10 HSO4- 11 OH- 12 HCO3. 13 CO3= 14 CO2 (d) 15 CaCO. 17 B(OH. 18 B(OH. 19 B3O3) 19 B3O3	- 	Ca++ Mg+H KgOH+ H+ SO4= - OH- HSO4- - OH- HSO4- CO2 (aq) CaC2 (aq) MgCO3 (aq) B(OH) 3 (aq) B(OH) 4- B3O3 (OH) 4-	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8 148.4	80 -2 05 -1 12 -2 08 -3 53 -3 66 -3 07 - 10 -1 10 -2 10 -1 89 -4 14 -4 32 -3 39 -4 57 -5	.83.468 (51.940 0.000 (52.955) (00.386 (04.942 (63.435) (36.751) (12.944 (55.680) (103.155) (103	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH- 7 H+ 8 C1- 9 S042 10 HS042 11 OH- 12 HC03- 13 C03= 14 C02 (d 15 CaC0) 17 B(OH) 18 B(OH) 19 B303 20 B405	- (aq) (aq) 3 (aq) 4- (OH) 4- (OH) 4=	Ca++ Mg0H+ Hg0H+ C1- SO4= HSO4- OH- HCO3- CO2(aq) CC2(aq) CC2(aq) MgCO3(aq) B(OH)3(aq) B(OH)4- B303(OH)4=	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 61.0 66.0 44.0 100.0 84.3 61.8 78.8 148.4 148.4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$.83.468 (51.940) 0.000 (52.955) (00.386 (04.942) (63.435) (36.751) (32.944) (35.680) (43.500) (43.500) (43.500) (13.155) (90.810) (65.200) (63.770) (39.100)	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH- 7 H+ 8 C1- 9 504= 10 H504- 11 OH- 12 HC03- 13 C03= 14 C02(15 16 MgC0) 16 MgC0 16 MgC0 16 B303 20 B405(1 20 B405(1)	- (aq) (aq) (aq) (aq) (a- (OH) 4- (OH) 4- (OH) 4- (OH) 4-	Ca++ MgoH+ HgOH+ C1- SO4= C03- C03- C03- C02(aq) MgC03(aq) MgC03(aq) B(OH)3(aq) B(OH)4- B3O3(OH)4- B4O5(OH)4+	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 1.0 35.4 96.0 97.0 17.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8 148.4 191.2 118.9	80 -2 505 -1 12 -2 508 -33 507 -33 507 -33 509 -23 107 -13 899 -4 14 -4 32 -33 339 -4 57 -52 66 -12 19 -6	.83.468 (51.940 0.000 (52.955) (00.386 (04.942) (63.435) (36.751) (12.944) (55.680) (43.500) (13.155) (143.500) (13.155) (143.500) (143.	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 7 H+ 8 Cl- 9 504= 10 HS04- 11 0H- 12 HC03- 13 C03= 14 C02(4 15 CaC0) 16 MgC0 17 B(0H) 18 B(0H) 19 B303 20 B405 21 CaB((22 MgB(0	- (aq) (aq) (aq) (aq) (a- (OH) 4- (OH) 4- (OH) 4- (OH) 4-	Ca++ Mg+H MgOH+ H+ Cl- SO4= HSO4- CO3= CO2 (aq) MgC03 (aq) B(OH) 3 (aq) B(OH) 3 (aq) B(OH) 3 (aq) B(OH) 4 B303 (OH) 4+	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8 148.4 148.4 191.2 118.9 103.1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$.83.468 (51.940 0.000 (52.955) (00.386 (04.942 (63.435) (36.751) (12.944) (55.680) (13.155) (143.580) (103.155) (143.580) (103.155) (143.580) (103.155) (103	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH4 7 H+ 8 Cl- 9 SO4= 10 HSO4- 11 OH- 12 HCO3- 13 CO3= 14 CO2((15 CaCO) 16 MgCO 17 B(OH) 18 B(OH) 18 B(OH) 19 B3O3 20 B4O5 21 CaB((22 MgB(O 23 Br-	- (aq) (aq) 3 (aq) 4- (OH) 4- (OH) 4= H) 4+ DH) 4+	Ca++ Mg0H+ Mg0H+ H+ Cl- SO4= OH- HC03- CO3= CO2(aq) CC03(aq) B(OH)3(aq) B(OH)4(aq) B(OH)4= B303(OH)4= CaB(OH)4+ BT-	aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 61.0 66.0 44.0 100.0 84.3 61.8 78.8 148.4 191.2 118.9 118.9 103.1 79.9	$\begin{array}{cccccccccccccccccccccccccccccccccccc$.83.468 (51.940) 0.000 (52.955) (00.386 (04.942) (63.435) (36.751) (12.944) (13.155)	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 Mg0H- 7 H+ 8 Cl- 9 SO4= 10 HSO4- 11 OH- 12 HCO3- 13 CO3= 14 CO2 (4 15 CaCO) 16 MgCO3 17 B(OH) 18 B(OH) 19 B3O3 20 BCO4 21 CaB((22 MgB((23 Br- 24 Clo4-	(aq) (aq) 3 (aq) 4- (OH)4- (OH)4- (OH)4- 2H)4+ 2H)4+ 2H)4+	Ca++ Mg++ HgOH+ H+ Cl- SO4= OH- CO2= CO2= CO2= (aq) MgCO3(aq) B(OH)3(aq) B(OH)4- B3O3(OH)4- B3O3(OH)4- CaB(OH)4+ MgB(OH)4+ Br- CaB(OH)4+ MgB(OH)4+ Br-	aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8 148.4 191.2 118.9 103.1 79.9 99.4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$.83.468 (51.940 0.000 (52.955) (00.386 (04.942 (63.435) (36.751) (12.944) (55.680 (143.500) (13.155) (190.810) (165.200) (165.	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 7 H+ 8 Cl- 9 504= 10 HS04- 11 0H- 12 HC03- 13 C03= 14 C02(4) 15 Ca(C) 16 MgC0 17 B(0H) 19 B303 20 B405 21 CaB(6) 22 MgB(0) 23 Br- 24 Cl04- 5 NaOH	(aq) (aq) 3(aq) 3(aq) 4- (OH)4- (OH)4- OH)4- 2H)4+ 2H)4+ 2H)4+ 2H)4+ 2H)4+ 2H(aq)to.titrate	Ca++ Mg+H Hg-Cl- SO4= HSO4- CO3= CO2 laq) MgCO3 (aq) B(OH) 3 laq) B(OH) 3 laq) B(OH) 4- B3O3 (OH) 4- B3O3 (OH) 4+ MgB(OH) 4+ Br- crate Clo4- .base.only	aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8 148.4 191.2 118.9 103.1 79.9 99.4 39.9	80 -2 80 -2 51 -2 52 -2 53 -3 53 -3 56 -3 57 -2 66 -3 7 -2 7 -2 7 -2 10 -3 89 -4 14 -4 32 -3 39 -4 57 -5 66 -12 19 -6 44 -6 51 -5 51	.83.468 (51.940) 0.000 (52.955) (00.386 (04.942) (63.435) (36.751) (12.944) (13.155)	
1 H2O 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH 7 H+ 8 Cl- 9 SO4= 10 HSO4- 11 OH- 12 HCO3- 13 CO3= 14 CO2((15 CaCO) 16 MgCO 17 B(OH) 18 B(OH) 18 B(OH) 19 B3O3 20 B4O5 21 CaB((22 MgB((23 Br- 24 ClO4+ 25 NaOH 26 HCl(((aq) (aq) 3(aq) 	Ca++ Mg0H+ Mg0H+ Cl- SO4= CO2 CO3= CO2[aq] CC2[aq] CC2[aq] B(OH)3[aq] B(OH)3[aq] B(OH)3[aq] B(OH)4= B303(OH)4= CaB(OH)4+ MgB(OH)4+ MgB(OH)4+ SrateClO4- stateClO4- cabase.only .acid.only	aqueous aqueous	40.0 24.3 41.3 1.0 55.4 96.0 97.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8 148.4 191.2 118.9 103.1 79.9 99.4 39.9 39.9	80 -2 55 -1 12 -2 08 -3 53 -3 56 -3 07 -2 17 -2 17 -2 10 -1 89 -4 32 -3 39 -4 57 -5 56 -12 19 -6 04 -9 51 -5 97 -5 51 -5 57 -5	.83.468 (51.940 0.000 (52.955) (00.386 (04.942) (63.435) (36.751) (12.944) (55.680) (13.155) (143.500) (13.155) (143.500) (13.155) (143.500) (155.200) (155.	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 MgOH4 7 H+ 8 Cl- 9 SO4= 10 HSO4- 11 OH- 12 HCO3- 13 CO3= 14 CO2(4 15 CaC0) 16 MgCO 17 B(OH] 18 B(OH) 19 B3O3 20 B405 21 CaB((22 MgB((22 MgB(C) 23 Br- 24 ClO4- 25 NaOH 26 HCl(7) 7 HclO- 7 HclO-	(aq) ((aq) 3 (aq) 3 (aq) 4- (OH) 4- (OH) 4- (OH) 4- 0H) 4+ - perchic (aq)to.titrate aq)to.titrate	Ca++ MgoH+ MgOH+ H+ Cl- SO4= OH- CO2 (aq) CC2 (aq) CC2 (aq) CC2 (aq) B(OH) 3 (aq) B(OH) 3 (aq) B(OH) 4 B3O3 (OH) 4- B3O3 (OH) 4- B3O3 (OH) 4- B3O3 (OH) 4- B3O5 (OH) 4- BT- mate Cl04- :base.only cacid.only	aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8 148.4 191.2 118.9 103.1 79.9 99.4 39.9	$\begin{array}{cccccccccccccccccccccccccccccccccccc$.83.468 (51.940) 0.000 (52.955) (00.386 (04.942) (63.435) (36.751) (32.944) (35.680) (43.500) (43.500) (43.500) (43.500) (43.500) (55.680) (43.500) (55.680) (43.500) (55.680) (43.500) (55.680)	
1 H20 2 Na+ 3 K+ 4 Ca++ 5 Mg++ 6 Mg0H4 7 H+ 8 Cl- 9 SO4= 10 HSO4- 11 OH- 12 HCO3 13 CO3= 14 CO2 (4) 15 CaC0 17 B(OH: 18 C) 18 B(OH: 18 B(OH: 18 B(OH: 18 B(OH: 18 B(OH: 18 C) 18 B(OH: 18 C) 18	(aq) (aq) 3(aq) 	Ca++ Mg0H+ H= Cl- SO4= HSO4- OH- CO2 aq) MgC03 (aq) B(OH)3 (aq) B(OH)3 (aq) B(OH)3 (aq) B(OH)3 (aq) B(OH)4- B303 (OH)4- B303 (OH)4- B405 (OH)4+ MgB(OH)4+ MgB(OH)4+ Br- trate Clo4- trate clo4-trate clo4-trate clo4-trate clo4-trate clo4-trate clo4-	aqueous aqueous	40.0 24.3 41.3 1.0 35.4 96.0 97.0 17.0 61.0 60.0 44.0 100.0 84.3 61.8 78.8 148.4 191.2 118.9 103.1 79.9 99.4 39.9 36.4	80 -2 80 -2 12 -2 13 -2 17 -2 10 -2 89 -4 14 -4 39 -4 57 -2 66 -12 19 -6 44 -6 51 -5 51 -5 59 -5 50 -5	.83.468 (51.940 0.000 (52.955) (00.386 (04.942) (63.435) (36.751) (212.944) (55.680) (43.500) (103.155) (90.810) (165.200) (16	

Appendix J: OUTPUT File Listing of HMW_NP_AM.CHEMDAT

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(343	31	. HNegIon(ag)to.titrate.acid	າຕາອຸດາ	s 1.00	500.000	
1311		Tracer(ag)conservative.tracer				
13.00		H3PO4 (ag) H3PO4 (ag)				
3/5		H2P04 H2P04				
1220	35	HP04* HP04=	aqueou			
12.2	36	PO4=- PO4=-	aqueou	s 94.972	-410.947	
1343	37	Np02+ Np02+	 aqueou aqueou 	s 269.041	-369.127	
(150) (160)	38	NpO2OH(ag) NpO2OH(ag)	aqueou		-438.518	
131 1	39	Np02(0H)2- Np02(0H)2-	aqueou aqueou	s 303.062	-505.829	
375	40	Np02003- Np02003-	aquéou	s 329.056	5 -594.492	
12.12	41	i P04=- P04=- Np02+ Np02+ Np02(q) Np02(q) Np02(q) Np02(q) Np02(q) Np02(q) Np02(q) Np02(q) Np02(q) Np02(q) Np02(c) Np02(c) Np02(c) Np02(c) Np02(c) Np02(c) Np02(c) Np02(c) Np02(c) Np02(c) Np02(c) Np02(c)	aqueou: aqueou:	s 329.056 s 389.065 s 449.075	-808,403	
	42	NDO2(CO3)3==- NDO2(CO3)3==-	aqueou	s 449.075	-1019.918	
1922	43	Am+++ Am+++ AmCO3+ AmCO3 Am(CO3)2- Am(CO3)2- Am(CO3)3=- Am(CO3)3=- Am(OH)2+ Am(OH)2+ Am(OH)2+ Am(OH)24	aqueou:			
- 1953 1953	44	AmCO3+ AmCO3+	aqueou:	s 303.009		
	4.5	Am(CO3)2= Am(CO3)2= Am(CO3)3=-	aqueou: aqueou:	s 363.018 s 423.028		
261	47	Am (OH) 2+ Am (OH) 2+		s 277.019		
100	48	Am (OH) 3 (ac) Am (OH) 3 (ac)	aqueou: aqueou:	s 294.022	-462.950	
	49	<i>Th++++</i> Th++++	aquecu.			
132	50	1102+4 11(371)02+4	3/714/011	c 770 079		
303	51	NoO2OH(aged) NoO2OH(aged)	eolid	286 054	-454.010	
1.1	52	NpO20H (gmc1) NpO20H (gmc1) NaNpO2CO3 (s) NaNpO2CO3 (s) Na3NpO2 (CO3) 2 (s) NANpO2CO3 (s)	solid	286.054	-452.642	
	53	NaNpQ2CO3(s)NaNpQ2CO3(s)	solid	352.046	-713.707	
1 A H S	54	Na3Np02(C03)2(s)_DISABLED_DISABLET	solid	458.035		
13-7	55	AmOHCO3(c) AmOHCO3(c) Am(OH)3(s) Am(OH)3(s)	solid	320.017		
10.65	56	Am (OH) 3 (S)Am (OH) 3 (S)	solid	294.022		•
- 1353 1873	57	hana((U))/2.012()(C)	solid	494.095		
- 10 - 1 - 10 - 1	20 50	NaAm(CO3)2.6H2O(c) AmPO4(c) AmPO4(c) CaSO4 NaK3(SO4)2Aphthitalite/Glaserite	5011G	337.972 136.138		
- 272	60	NaK3(504)2 Aphthitalite/Glaserite	solid	312 400	~1057.050	
	61	CaCl2 5820 Antarchicite	- solid	210 077		
10 M	62	CaCO3 Aragonite	solid	100.089		
11.1	63	K2504 Arcanite	solid	174.254		
1272	64	MgCl2.6H20Bischofite	solid	203.302	-853.100	
1272	65	CaC03 Aragonite K2S04 Arcanite MgC12.6H20 Bischofite Na2Ng(S04)2.4H20 Blocdite	solid	334.461		
1,72	66	Mg(OH)2Brucite	solid	58.320		
1373	67	Mg (OH) 2Brucite Na6CO3 (SO4) 2Burkeite CaCO3Calcite	solid	390.063		
1550) 1899 -	00 20	CaCl2_4H20CaCl2_Tetrahydrite	solid	100.089		
:332		Ca4Cl2(OH)6.13H20CaOxychloride A				
.2.27	71	Ca2Cl2(OH)2.H20 CaOxychloride B	solid	203.096		
1.114	72	KMgCl3.6H20Carnallite	solid	277.854		
ことう	73	MgSO4,7H20Epsomite	solid	246.465	-1157.830	
12.00	74	CaNa2(CO3)2.5H20Gaylussite	solid	296.154		
33	75	NMgCl3.6H20 Carnallite Mg504.7H20 Epsomite Cana2(CO3)2.5H20 Gaylussite Na22(SO4)2 Glauberite	solid	278.175		
1868 773	76	NaClGypsum NaClHalite	solid	172.168		
1.12	79	MacOA (V20 Vershudrite	solid	58.443 228.454		
13.1	79	MgS04.5H20Hexanyulite KMgCls04.3H20Kainite MgS04.H20Kalicinite K2Mg(s04)2.4H20Kieserite K2Mg(s04)3.2H20Labile_Salt	solid	248.960		
15.1	80	KHCO3Kalicinite	solid	100.115		
1393	81	MgSO4,H20 Kieserite	solid	138.378		
1304	82	K2Mg(S04)2.4H20Leonite	solid	366.678	-1403.970	
13.1	83	Na4Ca(SO4)3.2H20Labile_Salt	solid	456.242	-1751.450	
13.95	84	MgCO3Magnesite Mg2Cl(OH)3.4H2OMgOxychloride	solid	04.314		
1999	86	KHSO4Mercallite	solid	207.146 136.164		
1395	87	KHS04 Mercallite Na2S04.10H20 Mirabilite KBH6(S04)7 Misenite NaHC03 Nahcolite Na2C03.10H20 Natron MgC03.3H20 Nesquehonite K2Mg(S0412.6H20.Piccomertie/Schoon) Nesquehonite	solid	322.189		
:4: :	88	K8H6(SO4)7Misenite	solid	991.237	-3039,240	
. e." -	89	NaHCO3Nahcolite	solid	84.007	-343.330	
	90	Na2CO3.10H2ONatron	solid	286.141		
120-	91	MgCO3.3H20Nesquehonite	solid	138.360	-695.300	
14.54						
	93	Na2Ca(CO3)2.2H20Pirssonite K2MgCa2(SO4)4.2H20Polyhalite Ca(OH)2Portlandite	solid	242.108		
400	94	KAMGCa2(SO4)4.2H20Polyhalite	solid	602.922		
24 - 14 14 - 14	30	K2CO3.3/2H2OPotassium_Carbonate	solid	74.095 165.229		
		K8H4 (CO3) 6.3H2OFoctassium_carbonate		730,919		
121.)	98	KNaCO3.6H20K-Na-Carbonate	solid	230.188		
1411	99	K2NaH(CO3)2.2H20Potassium_Trona	solid	258.243		
		K3H(SO4)2Sesquipotassium_Sulfate		310.418		
		Na3H(SO4)2Sesquisodium_Sulfate		262.092	-919.600	
	102	Na2C03.7H20Na2C03-Heptahydrate	solid	232.095		
1416	103	KClSylvite K2Ca(SO4)2.H2OSyngenite	solid	74.551		
	104	K2Ca(SO4)2.H2OSyngenite Mg2CaCl6.12H2OTachyhydrite	solid	328.407		
1419	106	Na2504 Thenevelite	50110	517.590 142.037		
4.5	107	Na2504Thenardite Na2CO3.H20Thermonatrite	solid	124.004		
1225	108	Na3H(CO3)2.2H20Trona	solid	226.026		
1211	109	Na2B407.10H20Borax	solid	381.367		
: ? ; ; ;	110	Na2C03.H20	solid	61.832	-390,880	
	T T T	ABSU6.4HZUA-PencaDorace_(3V_C)	\$0110	293.204		
		K2B407,4H20K-Tetraborate_(30_C)		305.493		
523 5237	113	NaBO2.4H20Sodium_Metaborate NaB508.5H20Sodium_Pentaborate	solid	137.859		
	115	NaBSO8.5H20Sodium_Pentaborate NaBO2.NaCl.2H20Teepleite_(20_C)	solid	295.111 160.272		
1215			34114	100.272	- /23. //0	
1419						
:180		Truncated Name Formula Matr.				
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135	5	Mg++	0	0	٥	٥	1	0	0	0	٥	0	0	0	Q	0	0	0	0	0	0	0	0	02	
12		MgOH+	1	1	0	0	1	Ö	0	0	0	0	D	0	0	0	٥	0	0	0	0	Ô	0	01	
727	7	н+	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	٥	0	0	0	c	01	
	8	C1-	0	0	0	Q	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0 -1	
4.7		504=	0	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0 0	0	0	0	0	0 0	0 -2 0 -1	
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		CO2 (ag)	ō	z	ō	ō	ō	ō	ō	ō	ĩ	ō	Ō	ō	ō	ō	0	ō	ō.	ò	0	0	0	0 0	
		CaCO3 (ag)	o	3	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0 0	
·		MgCO3 (aq)	0	3	0	٥	1	0	0	0	1	0	0	0	٥	0	0	0	0	0	0	D	0	0 0	
2.5	17	B(OH)3(aq)	3	3	٥	٥	0	0	0	¢	0	0	D	0	1	٥	0	0	0	0	0	٥	0	0 0	
. 114		B(OH)4-	4	4	0	0	Û	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0 -1	
14		B303 (OH) 4-	4	7	0 0	0	0	0 0	0 0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0 -1 0 -2	
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1.1.5		MgB(OH)4+	4	4	ŏ	õ	1	ō	õ	ŏ	ō	ō	ō	ō	1	ŏ	ō	ō	ō	ō	ŏ	ō	ō	01	
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1252	24	C104- pe	0	Û	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	l	٥	0 -1	
120	25	NaOH(aq)to.ti	1	1	1	0	0	0	Ð	٥	0	0	0	٥	0	0	0	٥	0	0	0	0	0	0 0	
4		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	
		HC104 (aq) to.ti	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0 0	
145 459		Posion	0	0	0 0	0	0	0 0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0 1 0 - 1	
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1233		H3P04 (ag)	3	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0 0	
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. 4°.)		HPO4≠	1	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0 -2	
1400		PO4=-	0	4	0	Ó	0	0	0	0	0	0	0	0	0 0	0	0	0	0	0	0 1	0	1	0-3 01	
1417 1488		NpO2+	0	3	0 0	0	0	0 0	0 0	0	0 0	0	0	0	õ	0 0	0 0	0	õ	õ	1	õ	ō	0 0	
1243		NpO2OH(aq) NpO2(OH)2-	2	4	õ	õ	0	0	0	õ	õ	ő	ŏ	õ	õ	õ	õ	õ	ō	õ	1	õ	õ	0-1	
1.77		Np02C03-	õ	5	ō	õ	ō	ō	õ	ō	1	ō	ō	ō	ō	õ	0	0	0	ō	ī	ō	Ū	0 -1	
• • ?		NpO2 (CO3) 2=-	ō	8	Ó	ò	ō	Q	ō	ō	2	ō	ø	0	0	0	0	0	0	0	1	0	0	0 -3	
432	42	NpO2 (CO3) 3==-	0	11	0	0	0	0	0	0	3	0	0	0	0	0	0	D	0	Ô	1	0	0	0 -S	
A. 13		Am+++	0	0	0	0	0	0	0	D	0	0	0	0	0	٥	0	0	1	0	0	0	0	03	
		AmCO3+	0	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	01	
1473	45		0	6	0	0	0	0	0	0 0	2 3	0 0	0 0	0	0 0	0 0	0 0	0 0	1	0 0	0	0 D	0	0 ~1 0 -3	
47	46		0 2	9 2	0	0	0 0	0 0	0	ő	0	0	0	0	0	0	0	0	1	0	0	0	D	0 1	
473		Am (OH) 2+ Am (OH) 3 (aq)	3	3	õ	õ	0	ō	õ	õ	õ	õ	ŏ	ŏ	õ	õ	ŏ	ŏ	1	ŏ	ŏ	ŏ	ō	οō	
1477	49		ō	ō	ō	õ	õ	ō	ō	ō	ò	ō	ō	ō	¢.	ō	ò	1	D	ō.	¢.	0	D	04	
4.2		002++	0	2	0	ò	0	0	0	¢	0	0	0	0	0	0	0	0	0	1	0	0	0	02	
1481	51	NpO2OH(aged)	1	3	٥	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0 0	
: 451		NpO2OH(amor)	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0 0	
: 433		NaNp02C03(s)	0	5	1	0	0	0	0	0	1 2	0	0	0	0	0	0 0	0	0 0	0	1	0	0	00	
434 43		Na3NpO2(CO3)2(s)_DI AmOHCO3(c)	0	8	0	0	0	0	0	0	1	0 C	ō	õ	õ	õ	c c	ŏ	1	õ	ō	õ	õ	0 0	
جوني 1		Am(OH)3(s)	3	3	õ	õ	ō	ŏ	ŏ	0	ō	ŏ	ŏ	ŏ	0	õ	ŏ	õ	î	0	ō	ō	õ	οõ	
197	57	NaAm(CO3)2.6H2O(c)_	12		1	ō	õ	ō	ō	0	2	0	0	ο	0	0	0	Ó	1	0	0	σ	0	0 0	
1455	58	AmPO4 (c)	0	4	0	0	0	σ	0	C	0	0	0	0	0	0	0	0	1	0	0	0	1	0 0	
4.3 -	59	Ca504	o	4	٥	0	Ö	1	0	1	0	0	¢	0	0	Ð	0	0	0	0	0	0	0	0 0	
151		NAK3(SO4)2Aphthic	0	8	1	3	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	٥	0	00	
145		Cac12.6H20	12	6	0	0	0	1	2	0	0	0	0	0	0	0	0 0	0	0	0 0	0 0	0	C C	00	
1400 1400		Caco3 K2S04	0 0	3	0	2	0	2	0	0	1 0	0	0	0	0	0	0	0	ö	0	0	0	ō	00	
1292		MgC12.6H20	12	6	õ	é	1	ō	2	ċ	ő	ō	ŏ	ŏ	õ	ō	ō	ō	õ	ŏ	ŏ	õ	õ	õğ	
1847.		Na2Mg (SO4)2.4H20		12	2	ŏ	ĩ	ő	ō	2	ō	õ	ō	Q	ō	0	Ċ	Ō	o	0	0	٥	0	0 0	
. 4 (-0	66	Mg (OH) 2	2	2	0	0		٥	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0 0	
1437		Na6C03 (504) 2		11	6	Ö	0	0	0	ż	1	0	0	0	0	0	0	0	0	0	0	0	0	00	
1499 1499		CaC03CaC	0 8	3			0	1	0 2	0	1 0	0	0	0	0 0	0 0	0	0	0 0	0 0	0 0	0 0	0	0 0	
1600		Caci2, 4H20Cac Ca4ci2 (OH) 6.13H20						4	2	0	0	0	õ	0	0	0	0	0	õ	ō	0	õ	õ	0 0	
:5()	71	Ca2C12 (OH) 2. H20	4				ŏ	z	2					õ	ŏ	ō	ō	ō	ō	ō	ō	Ď		οĎ	
::::2	72	KMgC13.6H20	12				ì	ō	3		ō	ō	Ó	Ō	Ō	0	0	Ō	ò	0	0	0	0	οp	
÷513	73	MOCOA 7970	14	11	σ	ō	1	0		1		0	0	Ġ	0	0	0	0	0	Ô	0	0	0	0 0	
	74	CaNa2(CO3)2.5H20	10	11	2	0	0	1	0	-	2			0		0	0	0	0	0	0	0	0	0 0	
1606	75	Na2Ca (SO4) 2	0	8	2	0		1	0		0	0	0	0	0	0	0 0	0 0	0	0	0	0	0	0 0 0 0	
372	76	Caso4 .2H20	4	6	-	-		1	0	1		0		0		0 0	C C	0	č	0	0	Ď	0	-	
16.7 1818	79	MgS04,6H20	17	0	1	0	0 1	0	1 0	0	0 D		0	ő		0	0	0	ŏ	0	ō	0	0	0 D 0 D	
	79	KMgC1S04.3H20	-1-2 6	7	0	1	1	0	1				ō	ō		õ	ŏ	ō	õ	ŏ	õ			0 0	
1210		КНСО3		3			ō	ŏ	ō		1		ō	ō		ō	ō	ō	ō	Ó	0			0 0	
1511	81	MgS04.H20	2	5	0		1	ō			0	0	0	0	0	0		0	0	0	0		0	0 0	
1510	82	K2Mg(\$04)2.4H20		12					Ó				0	0		0	0	0	0	0	0		0	0 0	
12.13	83	Na4ca(SO4)3 2H20		14			0	1	0						0	0	0	0	0	0			0	0 0	
τ 4	84	MgC03		3			1	0		0				0		0	0	0 0	0 0	0	0		0 0	00 00	
17 19 19	80 84	Mg2C1 (OH) 3.4H20	¥ ۲.	4	0	0	2 0	0		0			0	0		0	ő	ö	0	ŏ	-		0 0	00	
	87	KHS04 Na2S04.10H20	20	14	2	ō	0	0		1		ō	ŏ	ō		õ	õ	ŏ	ō	ō	õ		ŏ	0 0	
1919	88	ዶ GH6 (SO4) 7	6	28	ō	8		õ		7					ō	õ			ō		ō		ō	0 0	
:4:49	89	NaHCO3		3		õ		ō	0	0	1	0	0			0	0	Q	0	0	0			0 0	
52.	90	N42CO3.10H20		13		-		0		0						0	0	0	0	0				0 0	
52		MgC03.3H20		6				0		0						0	0		0			0		0 0	
12.82	92	K2Mg(504)2.6H20 Pic	12	14	0	2	1	٥	0	2	0	Q	0	0	٥	0	٥	Ó	0	U	0	0	0	00	

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		Na2Ca (CO3) 2.2H20			4		÷	1	ž	ž	-	ž	ž	š	č	ž	ž	~	š	ž	Ä	Š.	~	ž	<u>~</u>
1501	94	K2MgCa2 (SO4) 4.2H2O_	4	18	0	z	1	2	Û	4	Q	0	U	0	0	U	0	U					U.	Ŭ,	
	95	Ca (OH) 2	2	Ż	0	0	0	1	0	0	0	0	¢	0	0	0	¢	0	Q	0	D	0	0	Q	0
820	96	K2C03.3/2H20Pota	3	4	0	2	0	D	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2 :		K8H4 (CO3) 6. 3H20K						0	0	0	6	0	0	0	0	0	0	Ô	C	0	0	0	0	0	0
·		KNaCO3.6H20			1	1	ò	0	0	٥	1	0	0	0	Ċ.	0	0	0	0	0	o	0	0	0	0
		K2NaH (CO3) 2.2H20			1	2	ō	ō	ò	0	2	o	o	0	0	0	0	0	0	0	0	0	0	0	0
3.3		K2NaH(CO3)2.2H20		ň	Â	5	Ň	-	~	-	ñ	ñ	ò	ō	ò	ñ	ò	٥	٥	0	n	n	n	٥	Ċ.
	100	K3H(SO4)2Sesquipo	÷.	ŝ	-	~	č	~	ž	5	Ä	~	ŏ	Ň	ň		Ā	-	Ā	Ā	Ā	ñ	ñ	ñ	ů.
		Na3H(SO4)2Sesqu				Q	0			2							ž	č	ž	č	ž		š	ž	
16.22	102		14			0	D	0	O	0	1	0	¢	0	0	U	Q	U	0	U	Ų.	0	0	0	U
:122	103	KC1	0	0	0	1	0	Û	1	0	0	0	0	¢	0	0	0	0	0	0	o	0	0	D	C
12.34	104	K2Ca(504)2.H20	2	9	0	2	0	1	0	2	0	0	0	0	0	Q	Û	0	D	0	0	0	0	0	0
	105	M. DO. 016 10000	24	12	0	0	2	1	6	0	0	0	Ô	٥	0	0	٥	٥	D	0	0	0	0	0	0
14145	106	Na2SO4	0	4	2	0	Q	0	Ð	1	0	0	0	0	D	٥	0	0	0	0	0	0	o	0	0
	107	Na2CO3.H20	2	4	2	0	0	0	C	0	1	Ô.	٥	0	0	0	0	0	0	0	0	0	0	0	0
1100	108	Na3H(CO3)2.2H20	5	8	з	0	Ð	0	C	0	2	0	0	0	0	0	0	0	0	0	¢	0	D	0	0
	100	Na2B407.10H20	20	17	2	ò	D	0	С	D	0	0	0	0	4	0	0	0	ð	0	0	0	0	٥	0
	103	B (OH) 3B	- 1	- i	0	ō	0	O.	с	٥	٥	Q	0	0	1	0	0	0	0	0	0	0	0	0	0
	110	KB508.4H20K-Pen	ŝ	12	ŏ	1	0	ò	c	0	D	0	0	ò	5	0	0	0	0	0	0	0	0	0	0
	111	KB508.4H20K-Fen			Ň	÷	ň	ň	ñ.	ň	ň	õ	ō	ō	ā	ō	ň	0	D	ò	٥	0	0	a	0
10-20	112	K2B407.4H20K-Tet	ŝ	÷+		4	š	č	~	Š	ž	ž	~	š		Ň	ŏ	ň	ň	Ā	ō	ň	5	ñ	0
		NaB02.4H20So						0	0	<u> </u>				0	-			2	2	Š	~	2	~	Ň	č
		NaB508.5H20Sod				0	0	o	0	0	0	0	0	0	5	a	0	0	0	0	0	0	0	0	0
$\epsilon \in \mathbb{C}$	115	NaB02.NaCl.2H20T	4	4	2	0	0	0	1	0	Ō	0	o	0	1	D	0	0	0	0	0	0	0	0	0
· · · · · ·			***	****	***	***	***	***	***	***	***	•••	• • •	***	***	***	***	***	***	***	• * *	***	***	***	*******



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

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

K.1 Listing

2

5 F (1) (1)

●日の●のなら日常ならせ日日できたとちがかかとなからないのでのないではないないのでもで、メメメルロション、 いた、ための日常になられたのではないないできた。このものでんどうでは、このでは、このでは、このではないで、このできんでいた。

See Table 25 for explanation of this listing.

2.43	Np(V)020H(aged)Np(V)020H(aged) *	
2.03	'Np(V)020H(amor),Np(V)020H(amor)'	
2.43	NaNp(V)02C03(s)NaNp(V)02C03(s)	
2.43	'NaNpO2CO3Na2CO3(s)Na3NpO2(CO3)2(s)'	
2.d3	AmoHCO3 (c)	
2.d3	Am (OH) 3 (S) NaAm (CO3) 2.6H2O (C)	
2.d3 2.d3	AmPO4 (c)	
\$.QJ	ALLE ON (C)	
2980.d0	CaSO4 Anhydrite	CRC p.B-181:185
2.d3	NaK3(504)2 Aphthitalite/Glaserite	
2.d3	CaCl2.6H2O Antarcticite	
2940.00	CaCO3 Aragonite	
2663.d0	K2SO4 Arcanite	CRC p.B-181:185
2.d3	MgCl2.6H2O Bischofite	
2250.d0		CRC p.B-181:185
2390.00		CRC p.B-181:185
2.43	Na6CO3(SO4)2 Burkeite	
2828.d0		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	000 - P 191-195
1602.d0		CRC p.B-181:185 CRC p.B-181:185
1677.d0 1991.d0	MgSO4.7H20 Epsomite CaNa2(CO3)2.5H20 Gaylussite	
2800.00	Na2Ca(SO4)2 Glauberite	
2335.00		CRC p.B-181:185
2165.d0	NaCl Halite	CRC p.B-181:185
2.d3	MgSO4.6H2O Hexahydrite	
2150.00		CRC p.E-181:185
2.63	KHCO3 Kalicinite	•
2571.d0		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
2.43	K8H6(SO4)7 Misenite NaHCO3 Nahcolite	
2.d3		
2.d3 2.d3	Na2CO3.10H2O Natron MgCO3.3H2O Nesquehonite	
2.03	K2Mg(SO4)2.6H20 Picromerite/Schoen	
2.03	NaZCa(CO3)2.2H2O Pirssonite	
2.d3	K2MgCa2(SO4)4.2H2O Polyhalite	
2.43	Ca(OH)2 Portlandite	
2.d3	K2C03.3/2H20 Potassium Carbonate	
2.d3	K8H4(CO3)6.3H2O K-Sequicarbonate	
2.43	KNaCO3.6H2O K-Na-Carbonate	
2.43	K2NaH(CO3)2.2H20 Potassium Trona	
2.d3	K3H(SO4)2 Sesquipotassium Sulfate	
2.43	Na3H(SO4)2 Sesquisodium Sulfate	
2.d3	Na2CO3.7H2O Na2CO3-Heptahydrate	
1990.00	KC1 Sylvite	CRC p.B-181:185
2.d3	K2Ca(SO4)2.H2O Syngenite	
2.43	Mg2CaCl6.12H2O Tachyhydrite	
2.d3	Na2SO4 Thenardite	CRC p.B-181:185
2255.d0 2140.d0	Na2CO3.H2O Thermonatrite Na3H(CO3)2.2H2O Trona	CRC p.B-181:185 CRC p.B-181:185
1715.d0	Na2B407.10H20 Borax	CRC p.B-181:185
2.03	B(OH)3 Borix Acid Solid	p.5 202,20J
2.03	KB508.4H20 K-Pentaborate (30 C)	
2.03	K2B407.4H20 K-Tetraborate (30 C)	
2.43	NaBO2.4H2O Sodium Metaborate	
2.43	NaB508.5H20 Sodium Pentaborate	
2.43	NaBO2.NaCl.2H2O Teepleite (20 C)	

K.2 References Cited in Listing

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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

Appendix L: Output File Listing of HMW_NP_AM.RHOMIN

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

MINERAL DENSITIES, KG/M^3, IN 1	FILE "RHUMIN"
NoO20H (aged) NoO20H (ag	red) 2000.00000000000
NpO2OH (aged) NpO2OH (ag NpO2OH (amor) NpO2OH (ar NaNpO2CO3 (s) NaNpO2CO3	nor) 2000.00000000000
NaNp02C03 (s) NaNp02C03	3(5) 2000.0000000000
Na3Np02(C03)2(s)_DISABLED_DISAB	BLED 2000.0000000000
AmOHCO3 (c) AmOHCO3	3(c) 2000.0000000000
AmOHCO3 (c) AmOHCO3 AmOHCO3 (c) AmOHCO3 Am (OH) 3 (s) Am (OH) 3 NaAm (CO3) 2 . 6H2O (c) Am (OH) 3	3(s) 2000.0000000000
Nahm(CO3)2_6H2O(c)	2000.00000000000
AmPO4 (c) AmPO4	(c) 2000.00000000000
AmPO4(c)AmPO4 CaSO4Anhydz	rite 2980.0000000000
NaK3 (SO4) 2Aphthitalite/Glaser	rite 2000.00000000000
CaCl2.6H20 Antarctic	ite 2000.00000000000
CaCO3Aragon K2SO4Arcar MgCl2.6H20Bischot Na2Mg(SO4)2.4H20Bloec	nite 2940.0000000000
K2SO4Arcar	nite 2663.00000000000
MgCl2.6H20Bischot	Eite 2000.00000000000
Na2Mg(S04)2.4H20Bloed	lite 2250.0000000000
Mg (OH) 2Bruc	ite 2390.00000000000
Na6C03(SO4)2Burke	ite 2000.0000000000
CaCO3Calo	ite 2828.0000000000
Na2R9 (504)2_422Bruc Na6C03 (504)2Bruc CaCl2_4H20CaCl2_Tetrahydr Ca4Cl2/0F16_13H20CaCperchlorid	ite 2000.00000000000
Ca4Cl2(OH)6.13H20Ca0xychlorid	le A 2000.00000000000
Ca2Cl2(OH)2.H20CaOxychlorid	le B 2000.0000000000
KMgC13.6H20Carnal1	Lite 1602.00000000000
Ca2C12 (0) 12 H20CaOxychlorid KMgCl3 6H20Carmall MgSO4 7H20Caoxychlorid KMgCl3 6H20Carmall MgSO4 7H20Cayluss Na2Ca (SO4)2_Gayluss Na2Ca (SO4)2_Gayluss Na2Ca (SO4)2_Gayluss KMgCl504 .H20Kair KHCO3Kaicir MgSO4 .H20_Kaiser K2Mg (SO4)2 .4H20_Leor Na4Ca (SO4)3 .2H20_Lebite_S Mg2Cl (OH)3 .4H20_MgOxychlor KHSO4_Mercall KH504_Me	nite 1677.00000000000 site 1991.0000000000
CaNa2 (CO3) 2.5H20Gay1055	rite 2800.00000000000
Nazca (SO4) zGrauber	2335.0000000000
Vacil Wall	lite 2165.00000000000
Macina	rite 2000.00000000000
KMmClsO4 3H20 Kair	ite 2150.00000000000
KHCO3 Kalicir	nite 2000.00000000000
MgSO4,H20 Kieser	ite 2571.00000000000
K2Mg(S04)2.4H20Leor	nite 2000.00000000000
Na4Ca(SO4)3.2H20Labile_S	alt 2000.00000000000
MgCO3Magnes	ite 3210.00000000000
Mg2Cl(OH)3.4H2OMgOxychlor	ide 2000.0000000000
KHS04Mercall	lite 2000.0000000000
Na2SO4.10H20MirabiJ	lite 1490.00000000000
KBH6 (SO4) 7AISER	ite 2000.000000000000000000000000000000000
NAHCO3NAHCO3	ron 2000.00000000000
Marcol 19420 Narchard	hite 2000.0000000000
KZMg(SO4)2.6H20 Picromerite/Sch	2000.00000000000
Na2Ca(CO3)2.2H2O Pirssor	ite 2000,00000000000
Na2Ca(CO3)2.2H20Pirssor K2MgCa2(SO4)4.2H2OPolyhal Ca(OR)2Portland	ite 2000.00000000000
Ca(OR)2Portland	Lite 2000.0000000000
K2CO3.3/2H2OPotassium_Carbon	ate 2000.0000000000
K8H4(CO3)6.3H20K-Sequicarbon	ate 2000.00000000000
KNaCO3.6H20K-Na-Carbon K2NaH(CO3)2.2H2OPotassium_Tz	ate 2000.00000000000
K2NaH(CO3)2.2H2OPotassium_Tz	ona 2000.00000000000
K3H(SO4)2Sesquipotassium_Sulf	ate 2000.0000000000
K3H(SO4)2Sesquipotassium_Sulf Na3H(SO4)2Sesquisodium_Sulf Na2CO3.7H2ONa2CO3-Heptahydr	ate 2000.0000000000
Na2CO3.7H20Na2CO3-Heptahydz	ate 2000.0000000000
KClSylv	rite 1990.0000000000
K2Ca (S04) 2. H20Syngen	lite 2000.0000000000
Mg2CaC16.12H2OTachyhydr	ite 2000.000000000000000000000000000000000
NazbugThenard	ite 2255.000000000000
Na3W(CO3)2 2H2O	ona 2140.000000000000
Na2B407 10H20 Po	arax 1715.00000000000
B(OH)3 Borix Acid So	lia 2000.0000000000
KB508,4H20 K-Pentaborate (30	_C) 2000.0000000000
K2B407.4H20 K-Tetraborate (30	
NaBO2.4H20Sodium Metabor	ate 2000.0000000000
Na2C03.7H20Na2C03-Heptahydy KC1Sylv KC2cs(504)2.H20Syngen Mg2CaCl6.12H20Tachyhydr Na2S04Thenard Na2C03.H20Thermonatz Na2H(CO3)2.2H20TT Na2H407.10H20Borix_Acid_Sc KB508.4H20K-Pentaborate_[30 KB508.5H20Sodium_Pentabor NaB02.4H20Tecpleite_[32	ate 2000.00000000000
NaBO2_NaCl.2H20Teepleite_(20	_C) 2000.0000000000



Appendix M: Sample Output File "BATCH_DOC.OUT"

Appendix M: Sample Output File "BATCH_DOC.OUT"

See Table 26 for explanation of this listing.

		e is Ul:[SCBABB.FMI							
2		is U1: [SCBABB.FMT							
		: is Ul:[SCBABB.FMT : is Ul:[SCBABB.FMT							
		•		ANN_NF_AR.CREMU	MI;1				
		rd Coded as 298.15K H_DOC.in; to illust		BATY'H' HURS		FMT V2.0			
7		FW86; Np(V)-Na-C03-				FM1 ¥2.Q			
		-Na-C1-C03-S04-P04			4.RRFF94)				
۰,				*					
5.1		• • • • • • • • • • • • • • • • • • • •		***********	*********	***********	************	• • • • • • • • • • • • • • • •	*********
		"CHEMDAT" FILE WOU	LD BE HERE ***						
- :	***	SEE APPENDIX J		**********					
÷.,									
- 22		ILITY PRODUCT VIOLA	TION	• •					
- 3	•• Mg (OH) 2	Brucit	e •• 1.00E+01	**					
<u>^</u> ?									
23		ILITY PRODUCT VIOLA							
01 00	** Mg2C1(OH)3.4H20	0MgOxychlorid	e •• 6.69E+00	••					
1	2 Solub	ility Product Viola	tions						
	Adding solid Mg(O)		Brucite						
25			85						
	1[.FD.TITRATE]BATCH	5_DOC.in; to illust			1	FMT V2.0			
ς.	DATABASE: HMW84/H	W86; Np(V)-Na-CO3-	OH-Cl-ClO4 (NR9-	4);					
÷.		-Na-C1-C03-S04-P04							
19	Pressure=	1.00000E+00 [=] AT	M Temperatu:	re= 2.96E+0	2 [=] Kelvin				
25	•••	(
21		es for Flash Probl	em						
	Total Moles	Aq. Molality	Aq. Molarity	Ag. mg/liter					
54									
35		Correlation							
20	1.10222364E+02	1.11116160E+02	1.10794086E+02	1.11669359E+0	5 Hydrogen			Constanting of the second	
<u>.</u> 27	5.51654821E+01	5.56118135E+01	5.54506206E+01	8.87176659E+0			نو ا	·	•
2 ک			2.01041045E-01	4.62188739E+0				The party	
22			1.00520523E-02	3.93018155E+0			۰.	· · · · · · · · · · · · · · · · · · ·	
\odot			4.63326856E-08	1.12611592E-0	•			- 1	
41			1.00520523E-04	4.02886254E+0					
42 ~?			1.10572575E-01 1.00520523E-03	3.92012950E+0 3.22268795E+0				· · · · ·	
~.	1.00000000E-03 1.00000000E-04		1.00520523E-04	1.20735200E+0					,
45	0.00000000E+00		0.0000000E+00	0.0000000E+0					
4÷,			0.0000000E+00	0.00000000E+0	0 Neglon				
61	0.0000000E+00	Q.0000000E+00	0.0000000E+00	0.0000000E+0	0 Air				
43			1.00520523E-07	1.08662685E-0					
~			0.0000000E+00	0.0000000E+0					
50	0.0000000E+00		0.00000000E+00	0.00000000E+0					
5 (5)	0.00000000±+00 0.000000000±+00		0.00000000E+00 0.0000000E+00	0.00000000E+0 0.00000000E+0					
53			0.00000000E+00	0.00000000E+0					
14	0.0000000E+00		0.0000000E+00	0.0000000E+0					
::	0.00000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+0	0 C104-(EL)				
2.5			0.0000000E+00	0.0000000E+0		s			
5.	0.0000000E+00		0.0000000E+00	0.00000000E+0					
55 59		4.94592698E-17	4.93159103E-17	0.00000005+0	o Charge				
<u>د</u>		ere Calculated							
(i		1002.5997610554	2 grams						
	H20 MASS	991.93820129674							
-00		10.748209661391							
- i a									
6.	Specified Soluti								
(()		1007.8185190420	2 kg/m^3 =	g/1					
2 - 2 - 2 - 2 - 2		ers Based on Speci.	fied Depeity						
- 65		0.99482172842828							
20		10.717055582938							
1									
12		TDS and NaCl solu		1851904202	ġ/l				
13		error vs NaCl den	sity 0.00000	000000000E+000	8				
. 4.									
?									
20 20		TIONS FOR BATCH SY	STEM						
	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
10	-							-	-
	H20	WATER	9.92444E-01	9.93023E-01	1.001	5.50612E+01	5.53478E+01	9.97101E+05	
3	Na+	Na+	2.01625E-01	1.47085E-01	0.7295	2.00000E-01	2.01041E-01	4.62189E+03	

/* · · .

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mondix M: S	ample Output File '	BATCH DO	C OUTT'		·			Page 14
ppendix M. S.								
	C1-	1.10894E-01	7.98916E-02	0.7204	1.10000E-01	1.10573E-01	3.92013E+D3	
2H-	OH-	9.87965E-02	7.13753E-02	0.7224	9.80001E-02	9.851022-02	1.67539E+03	
<+	K+	1.00813E-02	7.34149E-03	0.7282	1.00000E-02	1.00521E-02	3.93018E+02	
504 <i>=</i>	SO4=	1.00813E-03	2.24998E-04	0.2232	1.00000E-03	1.00521E-03	9.65576£+01	
g(OH)2		1.00808E-03	1.00000E+00	1.000	9.99954E-04	1.00516E-03	5.86205E+01	
3++	Ca++	1.00115E-04	2.00966E-05	0.2007	9.93083E-05	9.98252E-05	4.00099E+00	
)3=	CO3=	1.00005E-04	2 44915E-05	0.2449	9.91991E-05	9.97155E-05	5.98385E+00	
(OH) 4-	B(OH)4~	1.00709E-07	6.61270E-08	0.6566	9.98971E-08	1.00417E-07	7.91680E-03	
203 (ag)	CaCOJ (aq)	6.97236E-07	6.97236E-07	1.000	5.92615E-07	6.95215E-07	6.95835E-02	1.38E-10
:03-	HC03 -	1.10094E-07	7.499232-08	0.6812	1.09206E-07	1.09775E-07	6.69815E-03	1.60E-10
OH+	MgOH+	3.54268E-08	2.81647E-08	0.7950 0.2332	3.51412E-08 1.08988E-08	3.53241E-08	1.45932E-03	-2.47E-07
** <u> </u>	Mg++	1.09873E-08 8.72370E-11	2.56221E-09	0.6810		1.09555E-08	2.66273E-04	2.36E-10
B (OH) 4+	CaB(OH)4+ MgCO3(ag)	5.32206E-11	5.94047E-11 5.32206E-11	1.000	0.65337E-11 5.27915E-11	8.69841E-11 5.30663E-11	1.03441E-05	3.87E-11
2C03 (aq)	B(OH)3(aq)	1.65411E-11	1.61858E-11	0.9785	1.64077E-11	1.64931E-11	4.47424E-06 1.01980E-06	3.15E-10
OH)3(ag)	5(0H)5(8Q) H+	1.93212E-13	1.40201E-13	0.7256	1.91654E-13	1.92652E-13	1.94173E-10	1.62E-10 1.36E-10
7/2-1	CO2 (ag)	2.21142E-14	2.30277E-14	1.041	2.19360E-14	2.20501E-14	9.70422E-10	3.16E-10
2 (ag) B (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
04-	HSO4-	4.06799E-15	3.00314E-15	0.7382	4.03519E-15	4.05620E-15	3.93717E-10	2.03E-10
4012(08)6 13820	0CaOxychloride A	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.27E+01
16 (SO4) 7	Misenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+02
	Tetraborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.56E+01
	Pentaborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.79E+01
) H) 3	Borix Acid Solid	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.000002+00	-1.08E+01
2B407.10H20	Borix_Acid_Solid Borax	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.16E+01
H(CO3)2.2H20	Ттола	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.32E+01
CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.76E+00
SO4	Thenardite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.03E+00
2CaC16.12H20	Thenardite Tachyhydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	~4.59E+01
a (504) 2 H20	Syngenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.82E+00
1	Syngenite Sylvite	0.00000£+00	1.00000E+00	1.000	0.0000E+00	0.00000E+00	0.00000E+00	-4.13E+00
2C03.7H20Na	a2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.84E+00
3H(SO4)2Ses	squisodium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.18E+01
(SO4)2_Sesqui	ipotassium_Sulfate	0.000002+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+01
aH(CO3)2.2H20	Potassium_Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000£+00	0.0000E+00	-1.81E+01
CO3 . 6H20	K-Na-Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.48E+00
соз.3/2н20Ро	K-Na-Carbonate otassium_Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000£+00	0.00000E+00	0.00000E+00	-1.19E+01
10211	Portlandite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.80£+00
1gCa2 (SO4) 4.2H2	20Polyhalite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.31E+01
2Ca(CO3)2.2H2O_	Pirssonite	0.00000E+00	1.00000E+00	1.000	0.000002+00	0.00000E+00	0.00000E+00	-6.35E+00
Ig (SO4) 2.6H20 1	Picromerite/Schoen	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.58E+01
03.3н20	Nesquehonite	0.00000E+00	1.00000£+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.04E+00
.CO3.10H20	Natron Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.48E+00
ICO3	Nabcolite	0.00000E+00	1.00000E+00	1.000	0.DODDDE+00	0.00000E+00	0.00000E+00	-7.55E+00
	_Sodium_Metaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.35E+00
2SO4.10H20	Mirabilite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.12E+00
04	Mercallite MgOxychloride	0.0000E+00	1.00000E+00	1.000	0.0000E+00	0.00000E+00	0.00000E+00	-1.72E+01
.C1 (OH) 3.4H20_	MgOxychloride	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.77£+00
	Magnesite	0.0000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.37E+00
4Ca(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
1g(SO4)2.4H20_	Leonite	0.00000E+00	1.00000E+00	1.000	0.0000DE+00	0.00000E+00	0.00000E+00	-1.62E+01
504.H20	Kieserite	0.00000E+00	1.00000E+00	1.000	0.0000E+00	0.0000E+00	0.00000E+00	-1.21E+01
.03	Kieserite Kalicinite	0.00000E+00	1.00000E+00	1.000	0.0000E+00	0.00000E+00	0.00000E+00	-9.54E+00
CISO4.3H2O	Kainite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+60	-1.53E+01
ю4.6н20	Hexahydrite	0.000002+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.06E+01
<u></u>	Halite Gypsum	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.50E+00
504.2H20	Gypsum	0.00000E+00 0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.000000000000	0.00000E+00 0.00000E+00	-3.77E+00
2C4(SO4)2	Glauberite		1.00000E+00 1.00000E+00	1.000	0.00000E+00	0.00000E+00		-8.41£+00
		0.00000E+00		1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.18E+00
	Epsomite	0.00000E+00	1.00000E+00	1.000	0.0000E+00 0.00000E+00	0.00000E+00	0.000008+00	-1.04E+01
IgC13.6H20	Carnallite	0.00000E+00	1.00000E+00			0.00000E+00	0.00000E+00	-1.84E+01
	CaOxychloride B	0.00000E+00	1.00000E+00	1.000	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	-1.24E+01
	CaCl2_Tetrahydrite	0.00000E+00	1.00000E+00	1.000		0.00000E+00	0.00000E+00	-1.26E+01
CO3	Calcite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.02E-01
6CD3 (SO4) 2	Burkeite	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	-1.61E+01
2Mg (SO4) 2.4H2O			1.00000E+00	1.000	0.000002+00		0.00000E+00	-1.52E+01
	Bischofite	0.00000E+00 0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-1.53E+01
:504	Arcanite	0.00000E+00	1.00000E+00	1,000	0.000002+00	0.00000E+00	0.00000E+00	-6.14E+00
C03 C12_6H20	Aragonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.09£+00
	Antarcticite	C.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.11E+01 -1.07E+01
IK3 (SO4) 2April ISO4		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00		
	Anhydrite		1.00000E+00	1.000	0.000002+00	0.00000E+00	0.00000E+00	-3.98E+00
	Teepleite_(20_C)	0.00000E+00 0.00000E+00	1.00000E+00		0.00000E+00	0.00000E+00	0.00000E+00	-1.15E+01
	Sodium_Pentaborate		1.00000E+00	1.000	0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-4.782+01
	.titrate.base.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00		-2.93E+02
	.titrate.acid.only	0.00000E+00	0.00000E+00	0.1519	0.00000E+00		0.00000E+00	-2.54E+02 -3.36E+01
405 (OH) 4=	B405(OH)4≂ K-Semuicarbonate	0.00000E+00 0.00000E+00	1.00000E+00	1.000	0.000002+00	0.00000E+00 0.00000E+00	0.00000E+00	
8H4 (CO3) 6 . 3H2O 3O3 (OH) 4-	K-Sequicarbonate B3O3(OH)4-	0.00000E+00	0.00000E+00	0.5412	0.00000£+00	0.00000E+00	0.00000E+00 0.00000E+00	-6.18E+01 -2.70E+01
JUJ (UR) 4-	B303 [0R/ 4-	3.000002+00	5.00000±+00	0.3415	0.000000-00	5.0000E+00	5.0000E+00	-2.702+01
xmH ≈ -log[m(H+)] xH ≈ -log[a(H+)]] = = 12.8532	12.7140						
motic Coefficie								

(04 pH = -log[a(H+)] = 12.8532 100 Osmotic Coefficient= 0.919612 104 Equilibrium RK(%) = 99.302313 1057 Ionic Strength (m) = 0.213115 1059 Density, kg/m3 = 1007.82 1059 170 NOTES: - Water "molality" is mole fraction H20 in aqueous phase 171 - Gas "molality" and "activity" are gas partial pressures 172 - "Descriptor" means:

Appendix M: Sample Output File "BATCH_DOC.OUT"

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.73	*dG/RT/ln10 for species with	nonzero concs. (convergence criterion)
	"Saturation Index for minera	
177		species with very small concentrations
175	*log10(partial pressure) for	
132		
	Total G/RT= ~5.30370149E+03	
-	Total Diagonal Inversions 85	
101 1	Total Stoichiometric Reoptimizations	10

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Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

See Table 27 for explanation of this listing.

INPUT file name is U1: [SCBABB.FMT.USERGUIDE]NP_NACL_BM_LOG.IN:1	
INGUESS file name is Ul: (SCRABB.FHT.USERGUIDE) NP_NACL_BM_LOG.INGUESS:1	
OUTPUT file name is U1: (SCBABB.FMT.USERGUIDE)NP_NACL_EM_LOG.GUT:1 CHEMDAT file name is U1: [SCBABB.FMT.USERGUIDE]FMT_HHW_NP_AM.CHEMDAT:1	
Temperature is Hard Coded as 298.15K	
Benchmark TITRATE Problem. LOG10 option: Np(V)02 with CO3 in 5.61molal NaCl FMT V2.0	
DATABASE: HMWB4/FWB6; Np(V)-Na-CO3-OH-C1-C104 (NR94):	
95.01.31 Am(III)-Na-C1-C03-504-P04 (FRSR89,FRF90.P91,RFFR92,RFF94,RRFF94)	
· · · · · · · · · · · · · · · · · · ·	
· · · ECHO PRINT OF 'CHEMMAT' FILE WOULD BE HERE · · ·	
· ··· SEE APPENDIX J ····	
TITRATION Problem: -) Assigning all delta(y) to 0.1 m	
) Satisfield 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	
3	
RHONIN 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	
7 1.00E+00	
2 1.00E+00	
1.002+00 1.002+00	
1.00E+00	
4 1.00E+00 1.00E+00	
* inversions for batch pblm 50	
Benchmark TITRATE Problem, LOG10 option; Np(V)02 with CO3 in 5.61molal NaCl FMT V2.0	
2 DATABASE: HHW84/FW86; Np(V)-Na-CO3-CH-C1-ClO4 (NR94);	
3 95.01.31 Am(III)-Na-C1-C03-S04-P04 (FRSR89,PRF90,P91,RFF82,RFF94,RRFF94) 3 Pressure= 1.00000E+00 (=] ATM Temperature= 2.98E+02 (=] Kelvin	
Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin	
Elemental Abundances for Flash Problem	
3	
Total Moles Aq. Molality Aq. Molarity Aq. mg/liter	
1.11017363E+02 1.11029658E+02 1.00100314E+02 1.00891107E+05 Hydrogen	
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	
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g/kgH2O
                           306.214981877726
2.5
         TDS(c/kg)
9.1
       Specified Solution Density
                                                   kg/m^{3} = g/l
                           1177.63607439302
         DENSITY
 ÷ 1
 ž÷
       Solution Parameters Based on Specified Density
83
                           1.10906108219560
         SOLUTION VOL
                                                   liters
                           276.072326670473
                                                   g/l
         TOS
       Density based on TDS and NaCl solutions
                                                     1177.63607439302
                                                                             \sigma/1
23
                                                    0.000000000000000000000 %
       Percent relative error vs NaCl density
 4.2
 j,
 05
92
 1.
    TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
$ 3
                                                              Activity
                                                                             Act Coef
                                                                                           Total Moles Molarity
                                                                                                                          mg/liter
                                                                                                                                         Descriptor
                                               Molality
    Species Name
\frac{1}{2}
                                               8.57464E-01
                                                              8.59843E-01
                                                                               1.003
                                                                                           5.55025E+01
                                                                                                           5.00446E+01
                                                                                                                          9.01564E+05
                                    WATER
÷. *
    HZO
                                               5.61062E+00
                                                              3 69881E+00
                                                                             0 6593
                                                                                            5 61000E+00
                                                                                                           5 05833E+00
                                                                                                                          1 16290E+05
                                      Na+
•u:
    Na+
                                                                             2.05228-02
                                                                                           1.99385E+00
                                                                                                           1.79778E+00
                                                                                                                          1.07884E+05
                                     C03≄
                                               1 99407E+00
                                                              4.09214E-02
    C03=
                                                              1,06477E+00
                                               1.61018E+00
                                                                             0.6613
                                                                                            1.61000E+00
                                                                                                           1.45168E+00
                                                                                                                          5.14664E+04
in.
    C1-
                                      C1-
HCO3-
                                               6.14734E-03
                                                              1 59044E-03
                                                                             0.2587
                                                                                            6.14666E-03
                                                                                                           5.54222E-03
                                                                                                                          3.38170E+02
    HCO3-
                                                                                                           5.54221E-03
                                                                                                                          9.42580E+01
                                                                                                                                          2.00E-11
                                                                             0.7921
                                                                                            6.14665E-03
                                      OH---
                                               6 14733E-03
                                                              4.86901E-03
     OH-
                                                                              3.022
                                                                                                                                         -2.12E-07
-8.58E-08
                                               2.36876E-09
                                                              7.15913E-09
                                                                                            2.36850E-09
                                                                                                           2.13559E-09
                                                                                                                          9.39868E-05
-....>
                                  CO2 (ag)
    CO2 (ag)
                                               2.39954E-12
                                                              1.77959E-12
                                                                             0.7416
                                                                                            2.39927E-12
                                                                                                           2.16334E-12
                                                                                                                          2.18043E-09
    H+
                                                                                            0.00000E+00
                                                                                                           0.00000E+00
                                                                                                                          0.00000E+00
                                                                                                                                          -1.57E+00
                                                              1.00000E+00
                                                                               1,000
104
4 - 1
    Na3H(CO3)2.2H20_
                                    Trona
                                               0 00000E+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
                                                                                                                                          -2.92E+02
                                                                                                           0.000005+00
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.
     NaOH(aq)....to.titrate.base.only
                                               0.00000E+00
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11 <u>2</u>
• • • •
                                               0.00000E+00
     NaC1
                                   Halite
                               Nahcolite
                                               0.00000E+00
                                                              1.00000E+00
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                                                                                            0.00000E+00
                                                                                                           0.00000E+00
                                                                                                                          0.00000E+00
                                                                                                                                          -1.83E+00
    NAHCO3
                                                                                                                          0.00000E+00
- · 3
    Na2CO3.7H20____Na2CO3-Heptshydrate
                                               0.00000E+00
                                                              1.00000E+00
                                                                               1,000
                                                                                            0.000005+00
                                                                                                           0.00000E+00
                                                                                                                                          -2.51E+01
                                                                                            0.00000E+00
                                                                                                           0.00000E+00
                                                                                                                          0.00000E+00
                                                                                                                                          -7.99E-01
                                                                               1.000
Na2CO3 .H20_
                    Thermonatrite
                                               0.00000E+00
                                                              1.00000E+00
                                                                                            0.00000£+00
                                                                                                           0.00000E+00
                                                                                                                          0.00000E+00
                                                                                                                                          -8.30E-02
                                               0.00000E+00
                                                              1.00000E+00
                                                                               1,000
    Na2CO3.10H20_
                                  Natron
...
                                                 11.6199
----
    pmH = -log[m(H+)]
pH = -log[a(H+)]
11.7497
                          =
                              0.908418
:0
    Osmotic Coefficient=
•
    Equilibrium RH (%) =
Ionic Strength (m) =
                             85.984284
                              7.604695
122
                               1177.64
122 Density, kg/m3
•....
NOTES: - Water "molality" is mole fraction H2O in aqueous phase
             - Gas 'molality' and 'activity' are gas partial pressures
1.0
             - 'Descriptor' means:
                *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
-23
.....
                *Saturation Index for minerals, SI=log10(IAP/Ksp)
                *log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases
                    -6,42133776E+03
 ÷ •,
    Total G/RT=
134
121
                                        2.0000000000000000
                             1 sldsum
     Reaction #
     This is a solid-only reaction
:08
shifting left by
                         4 64434654478256
     calling makenuv for allomorphic reactions
# inversions for batch pblm 75
105-

        Internate TITRATE Problem, LOGIO option; Np(V)02 with CO3 in 5.61molal NaCl
        FMT V2.0

        PATABASE:
        HMM84/FW86; Np(V)-Na-CO3-OH-Cl-Cl04 (NR94);
        1%3
        95.01.31
        Am(III)-Na-Cl-CO3-S04-P04 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94)

ч/2
142
                                                                    2.98E+02 [=] Kelvin
•...•
                        1,00000E+00 [=] ATM
                                                  Temperature=
         Pressure=
1.44
     Elemental Abundances for Flash Problem
110
(7 )
                                            Aq. Molarity
                                                               Ag. mg/liter
164
                          Ag. Molality
       Total Moles
343
                                                               1.00169020E+05
                                                                                Hydrogen
· . .
       1.11018363E+02
                         1.11017591E+02
                                            9,93838868E+01
                                                               7.95078006E+05
                          5.55113597E+01
                                            4.96942389E+01
                                                                                Oxygen
       1.05508682E+02
       1.56100000E+01
                          5.61057382E+00
                                            5,02263316£+00
                                                               1 154691818+05
                                                                                Sodium
 :22
                                            0.0000000E+00
                                                               0.0000000E+00
                                                                                Potassium
 183
       0.0000000E+00
                          0.000000002+00
                          0.00000000E+00
                                            0.0000000E+00
                                                               0.000000002+00
                                                                                Magnesium
 144
       Calcium
 199
       0.0000000E+00
                          0.0000000E+00
                                            0.0000000E+00
                                                               0.0000000E+00
                                            5.02297975E+00
                                                               1.780797012+05
                                                                                Chlorine
 100
        5.61100000E+00
                          5.61096098£+00
                                             0.0000000E+00
                                                               0.0000000E+00
                                                                                Sulfur
                          0.0000000E+00
       0.0000000E+00
 100
100
100
                                                               6.58946152E+00
                          6.12839261E-04
0.0000000E+00
                                                                                Carbon
       1.0000000E+01
                                             5.486188922-04
                                            0.00000000E+00
                                                               0.0000000E+00
                                                                                Posion
       0.00000000E+00
                          0.0000000E+00
                                            0.0000000E+00
                                                               0.00000002+00
                                                                                Neglop
       0.0000000E+00
                                                               0.0000000E+00
 - 41
- 41
                                            0.0000000E+00
                                                                                Air
       0.0000000E+00
                          0.0000000E+00
                          0.0000000E+00
                                             0.0000000E+00
                                                               0.0000000E+00
                                                                                Boron
       0.00000000E+00
 0.0000000E+00
                          0.0000000E+00
                                            0.00000000E+00
                                                               0.00000002+00
                                                                                Bromine
                                             0.0000000E+00
                                                               0.0000000E+00
                                                                                TracerEl
       0.0000000E+00
                          0.00000000E+00
                          0.0000000E+00
                                             0.0000000E+00
                                                               0.0000000E+00
                                                                                Th(IV)
       0.0000000E+00
       0.0000000E+00
                                                               0.00000000E+00
                                                                                Am(III)
                          0.0000000E+00
                                             0.00000000E+00
                                             0.0000000E+00
                                                                                U(VI)
                          0.00000000E+00
       0.0000000E+00
 ÷ .....
       1.00000000E+01
                          6.12839261E-04
                                             5.48618892E-04
                                                               1.30049121E+02
                                                                                Np(V)
                                                               0.00000000E+00
                                                                                C104-{EL}
 1.55
        0.0000000E+00
                          0.0000000E+00
                                             0.0000000E+00
                                                               0.0000000E+00
                          0,0000000E+00
                                             0.00000000E+00
                                                                                Phosphorus
 121
       0,0000000E+00
                                            0.0000000E+00
                          0.0000000E+00
                                                               0 0000000E+00
                                                                                Electron
       0.0000000E+00
                        -2.37314981E-15 -2.12446380E-15
                                                               0.0000000E+00
                                                                                Charge
 :772
       -2.37316632E-15
```

• • •

		•	•						
:73									
174	Solution Parameter	rs, Calculated							
175	SOLUTION MASS	1328.11614865142	grams						
126	H20 MASS	1000.00695466819	grams						
· ? -	TDS(g/kg)	328.106912108529	g/kgH2O						
75									
	Specified Solution								
140	DENSITY	1188.93254605477	kg/m^3 =	g/1					
131									
32		s Based on Specifi							
182	SOLUTION VOL	1.11706602116201	liters						
1 <u>6</u> 4	TOS	293.724084134187	g/1						
345	Densing Lond on 1	TDS and NaCl soluti	one 1188 9	3254605477	g/l				
うか り 107		error vs NaCl densi		0000000000E+000					
122	fercent relative a								
182									
100									
:41	TABLE OF CONCENTRATI	IONS FOR BATCH SYST	'EM						
193	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
104									
	H20	WATER	8.31822E-01	7.77959E-01	0.9352	5.\$5091E+01	4.96918E+01	8.95208E+05	
т. 2		NaNp02C03(s)	9.99932E+00	1.00000E+00	1.000	9.99939E+00	8.95147E+00	3.15133E+06	
	C1-	C1-	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	
202		CO2 (ag)	3.86103E-04	1.12115E-03	2.904	3.86106E-04	3.45643E-04	1.52117E+01	
	HC03-	HCO3-	2.26571E-04	8.38810E-05	0.3702	2.26573E-04 1.33527 <i>E</i> -07	2.028298-04	1.237602+01	4.268-09
202 200	Np02C03-	Np02C03- H+	1.33526E-07 1.21872E-06	2.42971E-07 4.78095E-06	1.820 3.923	1.21873E-07	1.19534E-07	3.93334E-02	-1.99E-11
	н+ соз=	C03≠	3.09384E-08	8.03342E-10	2.5966E-02	3.09386E-08	1.09101E-06 2.76963E-08	1.09962E-03 1.66203E-03	-4.38E-08
	OH-	OH-	3.01685E-09	1.63977E-09	0.5435	3.01687E-09	2.70071E-09	4.59318E-05	-1.62E-07 2.55E-08
	Np020H (aq)	NpO2OH (aq)	7.72186E-10	7.72186E-10	1.000	7.72191E-10	6.91267E-10	1.97740E-04	1.87E-07
	Np02 (C03) 2=-	Np02 (C03) 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-	Np02 (OH) 2-	2.04382E-16	6.10703E-17	0.2988	2.04383E-16	1.82964E-16	5.54494E-11	2.13E-07
2.0	Np02 (C03)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
21)		Np020H(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.38£+00
211			0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000£+00	-2.99E+02
	HCl(aq)to.tit		0.00000E+00	0.00000E+00	1.000	0.00000€+00	0.00000E+00	0.00000E+00	-2.45E+02
	Na3Np02(C03)2(s)_DIS		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.36E+02
		Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.23E-01
	NaHCO3 Na2CO3.10H2O	Nahcolite Natron	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-2.95E+00 -7.91E+00
	Na2CO3.7H20Na2CO		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.95E+00
	Na2C03.H20	_Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.24E+00
	Na3H(CO3)2.2H20	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.02E+01
220	Np020H(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+00
Z ;									
	pmH = -log[m(H+)]	=	5.9141						
200		= 5.3205 1.241871							
225									
228	Ionic Strength (m) =								
227									
273									
229	NOTES: - Water "mol								
237		ity and activity	" are gas part	ial pressures					
221 232	- Descripto			(
2.0		0 for species with m Index for minera			circerion)				
2		ivity) for aqueous			centrations				
205		tial pressure) for	-						
222			-						
232		323084E+04							
	Flashing Titration #								A TANK
	<pre># inversions for bat</pre>		11					and the second s	A THE A
	1Benchmark TITRATE Pr				DIAL NACL F	MI V2.0		ALANCE.	
	DATABASE: HMW84/FW8 95.01.31 Am(III)-N				A REFEGAL			e contra	
242		00000E+00 [=] ATM	Temperatui		2 [=] Kelvin			- E	·· · ·
264								\$ S -	4 ·
	Elemental Abundances	for Flash Problem						· • .	
2.4.5									
347 243	Total Moles A	q. Molality Aq	. Molarity	Aq. mg/liter				Contrad . 30	
249	3.85857174E+01 1	11017591E+02 9.	93838868E+01	1.00169020E+0	5 Hydrogen		•	- E-4.2	1. June 1
250			96942389E+01	7.95078006E+0					
2.4			02263316E+00	1.15469181E+0					
2			00000000E+00	0.0000000E+0					
20%			00000000E+00	0.0000000E+0					
264			0000000E+00	0.0000000E+0					
265			02297975£+00	1.78079701E+0					
255			00000000E+00	0.0000000E+0					
2: 7 2: 7			48618892E-04	6.58946151E+0					
205			00000000E+00 00000000E+00	0.00000000E+0 0.00000000E+0					
200			00000000E+00	0.00000000E+0					
200			000000000E+00	0.00000000E+0					
24.2			00000000E+00	0.0000000E+0					

	Appendix N: Sar	npie Output rile	INP_INACI_BIN	1_LOG.001					
新和学校のなどの	0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 -6.94525850E-16 Solution Paramet	ers, Calculated	0.00000000E+00 0.0000000E+00 0.0000000E+00 5.48618892E-04 0.0000000E+00 0.0000000E+00 0.0000000E+00 -1.78886601E+15	0.00000000E+0 0.0000000E+0 0.0000000E+0 0.0000000E+0 0.0000000E+0 0.0000000E+0 0.0000000E+0	0 Th(IV) 0 Am(III) 9 U(VI) 2 Np(V) 0 ClO4-(EL) 0 Phosphorus 0 Electron	·			
275 275 275 275	SOLUTION MASS H2O MASS TDS(g/kg)	461,6021442510 347.5639950689 328.1069121081	56 grams						
078 114 220	Specified Soluti DENSITY	on Density 1188.932546054	59 kg/m.^3 ≃	g/1					
241 	Solution Paramet SOLUTION VOL TDS	ers Based on Spec: 0.3882492289262 293.72408413390	47 liters						
131 2947 2947		n TDS and NaCl solu error vs NaCl dem		3254603459 0000000000±+000	g/l %				
28-5 205 205	TABLE OF CONCENTRA	TIONS FOR BATCH ST	ISTEM						
20) 22)	Spaciac Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
<u>.</u>	Species Name		-	-			_	-	Descriptor
294 295	H20 NaNp02C03(s)	WATER NaNp02CO3(s)	8.31822E-01 9.99932E+D0	7.77959E-01 1.00000E+00	0.9352 1.000	1.92928E+01 3.47540E+00	4.96918E+01 8.95147E+00	8.95208E+05 3.15133E+06	
	c1-	C1-	5.61096£+00	5.29329E+00	0.9434	1.95017E+00	5.02298E+00	1.78080E+05	
	Na+ NpO2+	Na+ NpO2+	5.61057E+00 6.12705E-04	5.29268E+00 1.21978E-03	0.9433 1.991	1.95003E+00 2.12954E-04	5.02263E+00 5.48499E-04	1.15469E+05 1.47572E+02	
	CO2 (ag)	C02 (aq)	3.86103E-04	1.12115E-03	2.904	1.34196E-04	3.45643E-04	1.52117E+01	
	нсоз -	HCO3 ~	2.26571E-04	8.38810E-05	0.3702	7.87481E-05	2.028292-04	1.23760E+01	-6.17E-15
00	н+ Np02C03-	H+ Np02C03-	1.21872E-06 1.33526E-07	4.78095E-06 2.42971E-07	3.923 1.820	4.23582E-07 4.64090E-08	1.09101E-06 1.19534E-07	1.09962E-03 3.93334E-02	6.17E-15 1.85E-14
	C03=	€03≠	3.09384E-08	8.03343E-10	2.59662-02	1.07531E-08	2.76963E-08	1.66203E-03	0.00E+00
	OH-	OH- NDOZOH (aq)	3.01685E-09 7.72186E-10	1.63977 E -09 7.72186 E-1 0	0.5435 1.000	1.04855E-09 2.68384E-10	2.70071E-09 6.91267E-10	4.59318E-05 1.97740E-04	-6.17E-15 0.00E+00
	NpO20H(aq) NpO2(CO3)2=-	NpO2 (CO3) 2=-	1.983848-11	5.13355E-16	2.5877E-05	6.89511E-12	1.77595E-11	6.90960E-06	0.00E+00
207	NpO2 (OH) 2-	Np02 (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==- HCl(aq)to.t	NpOZ(CO3)3**-	1.25197E-16 0.00000±+00	9.87897E-26 0.00000E+00	7.8908E-10 1.000	4.35139E-17 0.00000E+00	1.12077E-16 0.00000E+00	5.03310E-11 0.00000E+00	-3.53É-10 -2.45É+02
31.5	NpO2OH(aged) NpO2OH(amor)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.38E+00
			0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+00
	NaOH(ag)to.t Na3NpO2(CO3)2(s)_I		0.00000E+00 0.00000E+00	0.00000E+00 1.00000E+00	1.000 1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-2.99E+02 -9.36E+02
			0.00000E+00	1.00000E+00	1.000	0.00000£+00	0.00000E+00	0.00000E+00	-1.23E-01
31:	NaHCO3 Na2CO3.10H20	Nahcolite	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1.000 1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-2.95E+00 -7.91E+00
	Na2C03.7H20Na2	Natron CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.95E+00
	Na2C03.H20	Thermonatrite	0.000002+00	1.00000E+00	1.000	0.0000E+00	0.00000E+00	0.00000E+00	-8.24E+00
219	Na3H(CO3)2.2H20	Trona	0.00000E+00	1.00000E+00	1.000	0.0000E+00	0.00000E+00	0.0000E+00	-1.02E+01
021	pmH = -log(m(H+))		= 5.9141						
	pH = -log[a(H+)] Osmotic Coefficien	= 5.3205 t= 1.241871							
	Equilibrium RH (%)								
225	Ionic Strength (m)	= 5.611188							
327	Density, kg/m3	= 1188.93		•					
12	NOTES: - Water "n								
- <u>2.2.)</u> 300		ality" and "activ. tor" means:	ity" are gas part	tial pressures					
30	*dG/RT/J	in10 for species w			criterion)				and any he has a second
322 323		ion Index for mine (ctivity) for aque			centrations			E. MONT	13
10		wartial pressure) :		very small con				ځ	
114		C-17001					-		S
	Total G/RT= -4. Flashing Titration	.63379813E+03							`, \$
	<pre># inversions for b</pre>		13						,
	<pre>lBenchmark TITRATE DATABASE: HMW84/F</pre>				DIAL NACI F	MT V2.0			
	95.01.31 Am(III)	-Na-C1-C03-S04-P0	4 (FRSR89, FRF90, 1	P91, RFFR92, RFF9					.
		1.00000E+00 [=] A	-	re= 2.98±+0	2 [=} Kelvin				
34. 3*: 54	Elemental Abundanc Total Moles	es for Flash Prob Aq. Molality	lem Ag. Molarity	Aq. mg/liter					
14					5 Wurdtenaar				
9439 2449	3.85957275E+01 3.66763098E+01	1.11017746E+02 5.55107903E+01	9.93891116E+01 4.96962723E+01	1.00174286E+0 7.95110540E+0					
	5.42594206E+00	5,61014105E+00	5.02250276E+00						
36 35	0.0000000E+00 0.0000000E+00	0.0000000E+00 0.0000000E+00	0.0000000E+00 0.0000000E+00	0.00000000E+0					

FMT, Version 2.0 User's Manual, Version 1.00

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Descriptor

-1.64E-12 -1.59E-11 -2.47E-14 2.55E-11 1.64E-11 -1.01E-11 2.65E-11

2.65E-11 -8.77E-11

-8.77E-11 6.38E-12 9.40E+00 -7.69E+00 -7.40E+00 -7.36E+00 -2.72E+00 -1.23E-01 -9.36E+02 -2.98E+02 -3.21E+00 -2.61E+00 -2.45E+02

•、 p

7	Appendix N: Sai	mple Output File '	"Np_NaCl_B!	M_LOG.OUT				
	• -							
53	0.0000000E+00		0.0000000E+00	0.0000000E+				
	1.95031318E+00		5.02231483E+00	1.78056128E+				
54. 50	0.00000000E+00 3.47579611E+00		0.00000000E+00 5.18560128E-04	0.0000000E+ 7.42952570E+				
;7	D.00000000E+00		0.0000000E+00	0.00000000E+				
į.	0.00000000E+00		0.0000000E+00	0.00000000E+				
3	0.0000000E+00		0000000E+00	0.0000000E+	•			
	0.00000002+00	0.0000000E+00 (00000000E+00	0.00000000E+	00 Boron			
1	0.0000000E+00		.00000000E+00	0.00000000E+				
κ.	0.0000000E+00		0.00000000E+00	0.0000000E+				
2	0.0000000E+00 0.0000000E+00		0.00000000E+00	0.00000000E+ 0.00000000E+				
5	0.000000002+00		.00000000E+00	0.00000000E+				
de la	3.47561578E+00		.54179484E-04	3.65479691E+				
27	0.0000000E+00		0.0000000E+00	0.0000000E+				
×.	0.0000000E+00		0.00000000±+00	0.00000000E+		s		
	0.00000000E+00 -7.46806759E-16		1.00000000E+00	0.00000000E+ 0.00000000E+				
÷	-/.46008/392-10			0.00000000000	ou charge			
	Solution Paramet	ters, Calculated						
3	SOLUTION MASS	461.665999617224						
<u>.</u>	H20 MASS	347.653675849716						
	TDS(g/kg)	327.947988724253	g/kgH20					
	Specified Soluts	on Density						
	DENSITY	1188.85111378691	l kg/m.^3 =	9/1				
¥			-	-				
		ers Based on Specif	-					
:	SOLUTION VOL	0.388329534508870						
2	TDS	293.596838859300	g/1					
	Density based or	TDS and NaCl solut	ions 1188.6	5111378 691	g/l			
τ.		error vs NaCl dens		0000000000E+00				
Û								
7								
j V		TIONS FOR BATCH SYS						
5	INDED OF CONCERNING	NTOND LOK DELON 315						
	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter
ά.								
	H20	WATER	8.31845E-01	7.78011E-01	0.9353	1.92978E+01	4.96944E+01	8.95254E+05
	NaNpO2CO3(s) Na+	NaNpO2CO3(s) Na+	9.99718E+00 5.61014E+00	1.00000E+00 5.29140E+00	1.000 0.9432	3.47556E+00 1.95039E+00	8.95002E+00 5.02250E+00	3.15082E+06
	C1-	C1-	5.60993E+00	5.29139E+00	0.9432	1.95031E+00	5.02231E+00	1.15466E+05 1.78056E+05
	HCO3-	HCO3-	3.82212E-04	1.41513E-04	0.3702	1.32878E-04	3.42177E-04	2.08787E+01
	C02 (ag)	CO2 (aq)	3.08476E-04	8.95671E-04	2.904	1.07243E-04	2.76165E-04	1.21539E+01
	Np02+	NpO2+	1.72085E-04	3.42481E-04	1.990	5.98258E-05	1.54059E-04	4.14492E+01
<u>0</u>		B+	5.77346E-07	2.26410E-06	3.922	2.00716E-07	5.16872E-07	5.20955E-04
	Np02C03-	Np02C03- C03=	1.33573E-07 1.10196E-07	2.43030E-07 2.86188E-09	1.819 2.5971E-02	4.64370E-08 3.83099E-08	1.19581E-07	3.93490E-02
	CO3= 0H-	OŊ-	6.37029E-09	3.46282E-09	0.5436	2.21466E-09	9.86531E-08 5.70303E-09	5.92010E-03 9.69932E-05
	NpO2OH(aq)	NDO2OH (ag)	4.57851E-10	4.57852E-10	1.000	1.59174E-10	4.09893E-10	1.17252E-04
	NpO2 (CO3)2=-	No02 (C03) 2=-	7.06677E-11	1.82925E-15	2.5885E-05	2.45679E-11	6.32656E-11	2.46144E-05
	NpO2(CO3)3≠≈-	NpO2(CO3)3=≈-	1.58546E-15	1.25406E-24	7.9097E-10	5.51192E-16	1.41939E-15	6.37413E-10
	NpO2 (OH) 2-	Np02 (OH) 2-	2.559032-16	7.646792-17	0.2988	8.89657E-17	2.29098E-16	6.94309E-11
	Na3H(CO3)2.2H20	Trona Thermonatrite	0.000002+00	1.00000E+00	1.000	0.000002+00	0.00000E+00	0.00000E+00
	Na2CO3.H20 Na2CO3.7H20Na2	COJ-Heptahydrate	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1.000 1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00
	Na2CO3.10H20	Nation	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
	NaHCO3	Nahcolite	0.00000E+00	1.000005+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
	NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
	Na3NpO2(C03)2(s)_D		0.0000E+00	1.00000E+00	1.000	0.00000E+0D	0.00000E+00	0.00000E+00
	NaOR(ag)to.t		0.000002+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
	NpO2OH(amor)	NpC2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
	NpO2OH(aged) HCl(aq)to.t		0.00000E+00 0.00000E+00	2.00000E+00	1.000	0.00000E+00	0.00000E+00	G.00000E+00
3	nc1(ag)	Atrace.acid.onty	0.00000£+00	Q.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
	pmH = -log(m(H+))	=	6.2386					
	$pH \approx -\log\{a(H+)\}$	= 5.6451						
	Osmotic Coefficien							
3	Equilibrium RH (%)	= 77.801108						
	Ionic Strength (m)							
	Density, kg/m3	≠ 1188.85						
0 7		clality is mole fr	action #20 in					A STATE OF
		ality and activit						
ē		tor means:						Ģ
0	*dG/RT/l	n10 for species wit			e criterion)			, er.,
1		ion Index for miner						· ·
		ctivity) for aqueou		very small co	ncentrations			
23 6	-log10(p	artial pressure) fo	r gases					ĩ
	Total G/RT= -4.	63438031E+03						
8 3	Flashing Titration	t ≢ 3						
7	inversions for b	atch pblm	22					
		Problem, LOG10 opti			molal NaCl 1	PMT V2.0		
2 I		W86; Np(V)-Na-CO3-O -Na-Cl-CO3-SO4-PO4			QA DEFEAL			
1. 1			LENSERY FRE90.		3% . KKFF94)			
40 ! 17 63		1.00000E+00 [*] ATM			02 [=] Kelvin			

.

Descriptor

-9.95E-12 -1.22E-10 8.21E-11 -1.23E-14 -8.04E-11 -1.14E-10

-1.14E-10 3.40E-11 -3.65E-07 -4.63E-11 -8.68E+00 -7.16E+00 -6.87E+00 -6.83E+00 -2.54E+00 -1.23E-01 -9.35E+02 -3.35E+00 -2.45E+02

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

443 Elemental Abundances for Flash Problem 444

4								
	Total Moles	Ag. Molality	Ag. Molarity	Ag. mg/liter				
440								
4.17	3.85999827£+01	1.11017943E+02	9.93906557 E+0 1	1.00175842E+05	5 Hydrogen			
468	3.66786675E+01	5.55109442E+01	4.96970938E+01	7.95123682E+05	5 Oxygen			
а ? С	5.42615710E+00	5.61002979E+00	5.02247225E+00	1.15465482E+05	5 Sodium			
	0.000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00) Potassium			
451	0.0000000E+00	0.0000000E+00	D.0000000E+00	0.0000000E+00) Magnesium			
482	0.0000000E+00	0.0000000E+00	0.00000000E+00	0.00000000E+00) Calcium			
452	1.95037489E+00	5.60950015E+00	5.02199808E+00	1.78044898E+05	5 Chlorine			
6.44	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00) Sulfur			
4	3.47587277E+00	7.90126088E-04	7.07373490E-04	8.49626299E+00	Carbon			
6	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00	> Posion			
407	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	Neglon			
452	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	Air			
45.1	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	Boron			
14.	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00) Bromine			
65.5	0.00000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00) TracerEl			
6.7	0.00000000E+00	0.0000000E+00	0.00000000E+00	0.00000000E+00				
40.5	0.0000000E+00	0.0000000E+00	0.00000000E+00	0.0000000E+00	Am(III)			
404	0.0000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				
105	3.47561578E+00	5.09860080E-05	4.56460697E-05	1.08203186E+01	L Np(V)			
<u> </u>	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00				
4	0.0000000E+00	0.00000000E+00	0.0000000E+00	0.00000000E+00	Phosphorus			
455	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00				
409			-4.77078632E-15	0.00000000E+00				
475-					-			
473	Solution Paramet	ers, Calculated						
472	SOLUTION MASS	461.7012242457	77 grams					
47.5	H20 MASS	347.6913876607	-					
4,	TDS(g/kg)	327,9052649308						
<u>.</u> 7								
470	Specified Soluti	on Density						
477	DENSITY	1188.829220713	61 kg/m^3 =	a/l				
177								
479	Solution Paramet	ers Based on Spec	ified Density					
dire)	SOLUTION VOL	0.3883663155323						
40:	TDS	293.5626289544						
322	-20		•					
483	Densiev based op	TDS and NaCl sol	utions 1188.82	2922071361	g/1			
46.		error vs NaCl de		000000000000000000000000000000000000000				
64.5								
47.7								
427								
428	TABLE OF CONCENTRA							
			YSTEN					
		CTIONS FOR BAICH S	YSTEM					
48.2		CTIONS FOR BRICH 3		Activity	Act Coef	Total Moles	Molarity	mg/liter
48.9 490	Species Name	CTIONS FOR BAICH S	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter
48.9 490 491	Species Name		Molality	-			_	•
489 490 491 492	Species Name H2O	WATER	Molality 8.31852E-01	7.78030E-01	0.9353	1.92999E+01	4.96951E+01	8.95267E+05
487 490 4452 493	Speciės Name H20 NaNp02C03(s)	WATER NaNpO2CO3(s)	Molality 8.31852E-01 9.99622E+00	7.78030E-01 1.00000E+00	0.9353	1.92999E+01 3.47560E+00	4.96951E+01 8.94928E+00	8.95267E+05 3.15056E+06
487 490 491 492 492 492 493	Species Name H2O NAMpO2CO3(s) Na+	WATER NaNpO2CO3 (s) Na+	Molality 8.31852E-01 9.99622E+00 5.61003E+00	7.78030E-01 1.00000E+00 5.290B0E+00	0.9353 1.000 0.9431	1.92999E+01 3.47560E+00 1.95056E+00	4.96951E+01 8.94928E+00 5.02247E+00	8.95267E+05 3.15056E+06 1.15465E+05
480 490 491 492 492 493 493 493 493 493 493	Speciės Name H2O NaNpO2CO3(s) Na+ Cl-	WATER NANpO2CO3 (s) Na+ C1-	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.60950E+00	7.78030E-01 1.00000E+00 5.290B0E+00 5.29073E+00	0.9353 1.000 0.9431 0.9432	1.92999E+01 3.47560E+00 1.95056E+00 1.95037E+00	4.96951E+01 8.94928E+00 5.02247E+00 5.02200E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05
4800 1 2 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	Speciės Name H2O NaNpO2CO3(s) Na+ Cl- HCO3-	WATER NANDO2CO3 (s) Na+ C1- HCO3-	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.60950E+00 5.79856E-04	7.78030E-01 1.00000E+00 5.29080E+00 5.29073E+00 2.14695E-04	0.9353 1.000 0.9431 0.9432 0.3703	1.92999E+01 3.47560E+00 1.95056E+00 1.95037E+00 2.01611E-04	4.96951E+01 8.94928E+00 5.02247E+00 5.02200E+00 5.19125E-04	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01
4800112334 499449334 49934 49934 49934 49934	Species Name H20 NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq)	WATER NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq)	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.60950E+00 5.79856E-04 2.09763E-04	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04	0.9353 1.000 0.9431 0.9432 0.3703 2.903	1.92999E+01 3.47560E+00 1.95056E+00 1.95037E+00 2.01611E-04 7.29329E-05	4.96951E+01 8.94928E+00 5.02247E+00 5.02200E+00 5.19125E-04 1.87794E-04	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00
48904452334459445544455	Species Name H20 NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+	WATER NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+	Molality 8.31852E-01 9.99622E+00 5.6103E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05	7.78030E-01 1.0000E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05	4.96951E+01 8.94928E+00 5.02247E+00 5.02200E+00 5.19125E-04 1.87794E-04 4.55260E-05	8.95267E+05 3.15056E+05 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01
800450000000000000000000000000000000000	Speciės Name H20 NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= CO3=	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO4- CO3=	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07	4.96951E+01 8.94928E+00 5.02247E+00 5.02200E+00 5.19125E-04 1.87794E-04 4.55260E-05 3.33916E-07	8.95267E+05 3.15056E+06 1.15465E+05 3.1675E+01 8.26478E+00 1.22486E+01 2.00380E-02
80011234 45934 45934 45034 4503 4503 4503 4503 4503 4503 4	Species Name H20 NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+	WATER NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+	Molality 8.31852E-01 9.99622E+00 5.6103E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05	7.78030E-01 1.0000E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05	4.96951E+01 8.94928E+00 5.02247E+00 5.02200E+00 5.19125E-04 1.87794E-04 4.55260E-05	8.95267E+05 3.15056E+05 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01
800450000000000000000000000000000000000	Species Name H20 NaP02C03(s) Na+ C1- HC03- C02(aq) Np02+ C03= H+ Np02C03-	WATER NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3 H+	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.6950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 2.58813E-07	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921	1.92999E+01 3.47560E+00 1.95056E+00 2.01611E-04 7.29329E-05 1.29682E-07 8.99871E-08	4.96951E+01 8.94928E+00 5.02247E+00 5.19125E-04 1.87794E-04 4.55260E-05 3.33916E-07 2.31707E-07	8.95267E+05 3.1505E+06 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.33537E-04
880112004 445004 45004 45004 4507 450900 102 500012	Speciės Name H20 NaHpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH-	WATER NANPO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3-	Molality 8.31852E-01 9.99622E+00 5.6103E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72379E-07 2.58813E-07 1.33591E-07	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08	4.96951E+01 6.94928E+00 5.02247E+00 5.19125E-04 1.87794E-04 4.55260E-05 3.33916E-07 1.19600E-07	8.95267E+05 3.15056E+06 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 3.3537E-04 3.93550E-02
8001200425975900020 8044590425975900020 80005975900020	Species Name H20 NaNp02C03(s) Na+ C1- HC03- C02(aq) Np02+ C03= H+ Np02C03- OH- Np02(C03)2=-	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2C03- H+ NpO2CO3- OH-	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 2.58813E-07 1.33591E-07 1.42123E-08	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436	1.92999E+01 3.47560E+00 1.95036E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09	4.96951E+01 6.94928E+00 5.02247E+00 5.02200E+00 5.19125E-04 1.87794E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.19600E+07 1.27238E-08	8.95267E+05 3.15056E+06 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.33537E-04 3.93550E-02 2.16397E-04
8991234 1875900 120 8991234 1875900 120 149500 100 100	Species Name H20 NahpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2OH(aq)	WATER NaNpO2CO3 (s) Na+ Cl- HCO3- CO2 (aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2 (CO3) 2=-	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 2.58813E-07 1.33591E-07 1.42132E-08 2.39201E-10	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11	4.96951E+01 8.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.27238E-08 2.14149E-10	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.33537E-04 3.93550E-02 2.16337E-04 8.33180E-05
800120040575900120045 80012004575900120045	Species Name H20 NaNp02C03(s) Na+ C1- HC03- C02(aq) Np02+ C03= H+ Np02C03- OH- Np02(C03)2=-	WATTER NANPO2CC3 (s) Na+ C1- HC03- C02 (aq) Np02+ C03= H+ Np02C03- OH- Np02 (C03) 2=- Np02OH (aq)	Molality 8.31852E-01 9.99622E+00 5.6103E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.7279E-07 2.58813E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000	1.92999E+01 3.47560E+00 1.95056E+00 2.01611E-04 7.29229E-05 1.76808E-05 3.99682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31663E-11 1.04942E-10	4.96951E+01 6.94928E+00 5.02247E+00 5.19125E-04 1.87794E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.19600E-07 1.27238E-08 2.14149E-10 2.70215E-10	8.95267E+05 3.15056E+06 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.16337E-04 8.33180E-05 7.72962E-05
8991234 187590 12045	Species Name H20 NaNp02c03(s) Na+ C1- HC03- C02(aq) Np02+ C03= H+ Np02C03- OH- Np02(C03)2=- Np02(C03)3==- Np02(C03)3==- Np02(C03)3=-	WATER NaNpO2CO3 (s) Na+ Cl- HCO3- CO2 (aq) NpO2 (cd) 2=- NpO2 (CO3) 2=- NpO2 (CO3) 2=- NpO2 (CO3) 3=-	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 1.33591E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 9.68710E-09 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.2932E+05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15	4.96951E+01 8.94928E+00 5.02247E+00 5.02200E+00 5.19125E-04 1.87794E+04 4.55260E-05 3.33916E-07 1.39600E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.0380E-02 2.33537E-04 3.93550E-02 2.16397E-04 8.33180E-05 7.29866E-09
4991234187590012034500 4991234187590012034500 5000012034500 50000	Species Name H20 Nah02C03(s) H20 H20 H20 Np02(03) H4 Np02C03- OH- Np02(03)2=- Np02(03)3=- Np02(03)3=- Np02(03)2.2H20 Np02(03)2.2H20	WATER NaNpO2CO3 (s) Na+ Cl- HCO3- CO2 (aq) NpO2 (co3) H+ NpO2CO3- OH- NpO2 (co3) 2=- NpO20H (aq) NpO2 (cO3) 3=- NpO2 (cO3) 3=-	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 2.58813E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29662E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7228E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.36963E-16	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.33537E-04 3.93550E-02 2.16397E-04 8.33180E-05 7.72962E-05 7.2966E-09 1.02121E-10
80012342875900223450078 804459342875900223450078 800249900223450078	Speciés Name H20 NaPpO2c03(s) Na+ C1- HC03- C02(aq) NpO2+ C03= H+ NpO2C03- OH- NpO2(C03)2=- NpO2(C03)2=- NpO2(C03)2=- NpO2(OH)2- Na3H(C03)2.2H20	WATTER NaNpO2C03 (s) Na+ C1- HC03- C02 (aq) Np02+ C03= H+ Np02C03- OH- Np02 (C03) 2=- Np020H (aq) Np02 (C03) 3=- Np02 (OH)2= Np02 (OH)2- Trona	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.7279E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888EE-05 1.000 7.9155E-10 0.2988 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.00000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.3916E-07 2.31707E-07 1.9600E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.69652E-16 0.00000E+00	8.95267E+05 3.15056E+06 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.16397E-04 8.33180E-05 7.72962E-05 7.29866E-09 1.02121E-10 0.00000E+00
8991264:5759000204500089 899444990000204500089 899444444990000204500089	Speciés Name H20 NaPpO2c03(s) Na+ C1- HC03- C02(aq) NpO2+ C03= H+ NpO2C03- OH- NpO2(C03)2=- NpO2(C03)2=- NpO2(C03)2=- NpO2(OH)2- Na3H(C03)2.2H20	WATER NaNpO2CO3 (s) Na+ Cl- HCO3- CO2 (aq) NpO2 (cd) 2=- NpO2CO3 (aq) NpO2 (CO3) 2=- NpO2 (CO3) 3==- NpO2 (CO3) 3=- NpO2 (CO3) 3==- NpO2 (CO3) 3=- NpO2 (CO3) 3=- NpO	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.03826E-10 1.43698E-23 1.12471E-16 1.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.00000E+00	4.96951E+01 8.94928E+00 5.02247E+00 5.0220E+00 1.87794E-04 4.55260E-05 3.33916E-07 1.31707E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.36963E+16 0.00000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.0380E-02 2.33537E-04 3.93550E-02 2.16397E-04 8.33180E-05 7.72962E-05 7.29866E-09 1.02121E-10 0.00000E+00
8991264:5759000204500089 899444990000204500089 899444444990000204500089	Species Name H20 NahpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)3=- NpO2(CO3)2=- NpO2(O3)3=- NpO2(CO3)2=- NpO2(C	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2(c) H+ NpO2CO3- HPO2(C3)2=- NpO20(aq) NpO2(C3)2=- NpO2(04)2=- NpO2(04)2=- Tronatrite 2CO3-Heptahydrate	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.8833E-07 1.3591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.07044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29662E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.00000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 1.87794E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.36963E-16 0.00000E+00 0.00000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.33537E-04 3.93550E-02 2.16397E-04 8.33180E-05 7.72962E-05 7.2966E-09 1.02121E-10 0.00000E+00 0.00000E+00
4001200445000000000000000000000000000000	Species Name H20 NahpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)3=- NpO2(CO3)2=- NpO2(O3)3=- NpO2(CO3)2=- NpO2(C	WATTER NaNpO2CO3 (s) Na+ Cl- HCO3- CO2 (aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2 (CO3) 2=- NpO2 (CO3) 3=- NpO2 (CO3) 3=- NpO2 (CO3) 3=- Trona Thermonatrite 2CO3-Heptahydrate Natron	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.7279E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76382E-15 0.00000E+00 0.00000E+00 0.00000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888EE-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64464E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 0.00000E+00 0.00000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.36963E-16 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+05 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.16397E-04 8.33180E-05 7.72962E-05 7.72962E-05 7.29866E-09 1.02121E-10 0.00000E+00 0.00000E+00
48901 4492 4492 4492 4999 4990 4990 500 200 4999 500 4995 500 500 500 500 500 500 500 500 500	Species Name H20 NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O3)3==- NpO2(O3)2=- NpO2(O3)3=- NpO2(O3)2=- Na2CO3.H2ONa2 Na2CO3.H2ONa2 Na2CO3.H2ONa2 NaC3	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CC2(a] NpO2 CO3= H+ NpO2(CO3)2=- NpO2	Molality 8.31852E-01 9.99622E+00 5.6103E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72379E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	7.78030E-01 1.0000E+00 5.29073E+00 2.14695E-04 6.39044E-04 1.01191E-04 9.68710E-09 1.01460E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29662E-07 8.99671E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-15 0.00000E+00 0.00000E+00 0.00000E+00	4.96951E+01 8.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 1.87794E-04 4.55260E-05 3.33916E-07 1.3960E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.36963E-16 0.00000E+00 0.00000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.0380E-02 2.33537E-04 3.93550E-02 2.16397E-04 8.33180E-05 7.29866E-09 1.02121E-10 0.00000E+00 0.00000E+00 0.00000E+00
4001 4400 4400 1000 1000 4600 1000 1000	Speciés Name H20 NahpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2.2H20Na2 Na2CO3.1H20Na2 Na2CO3.1H20Na2 Na2CO3.1H20Na2 Na2CO3.2H20NA2 Na2CO3.2H20 Na2CO3.2H20 Na2CO3	WATTER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3=- NpO3(CO3)3=	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.8833E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.75603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.993 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47550E+00 1.95037E+00 2.91611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.6444E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.02225-04 1.87794E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.36963E-16 0.00000E+00 0.00000E+00 0.00000E+00 0.0000DE+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.6755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.33537E-04 3.93550E-02 2.16337E-04 3.93550E-02 2.16337E-04 3.93550E-02 1.6277E-04 3.93550E-02 1.02121E-10 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 1.6277E-04 3.9565E-02 1.6277E-04 3.9575E-01 1.6277E-04 3.9575E-02 1.6277E-04 3.9575E-
4991 2994 2994 2995 2995 2995 2995 2995 2995	Speciés Name H20 NaPpO2CO3(s) Ne+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2(CO3)2=- NpO2(CO3)2=- NpO2(OH)2- NaO2(CO3)2.2H20Na2 Na2CO3.H20Na2 Na2CO3.10H20Na2 NaCO3_10H20Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NaCO3NA2 NACO3NA2 NAC	WATER NANPO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2(ca) H- NpO2CO3- H- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3=- Trona Thermonatrite CO3-Heptahydrate Natron Natron Natron Natron Natron Natron Natron	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72795E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76385E-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 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888EE-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 1.3960E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.36963E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+05 1.78045E+05 3.1675E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.16397E-04 8.33180E-05 7.72962E-05 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
8001 2004 2004 2000 2004 2001 2004 2004 2	Speciés Name H20 NahpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2.2H20Na2 Na2CO3.1H20Na2 Na2CO3.1H20Na2 Na2CO3.1H20Na2 Na2CO3.2H20NA2 Na2CO3.2H20 Na2CO3.2H20 Na2CO3	WATER NaNpO2CO3(s) NCC3- CO3- CO2(aq) NpO2(ca) NpO2(ca) NpO2(ca) NpO2(ca) NpO2(ca) NpO2(ca) NpO2(ca) NpO2(ca) NpO2(ca) NpO2(ca) NpO2(ca) Trona Thermonatrite CO3-Heptahydrate Natron Nahcolite Halite DISABLED_DISABLED Litrate,base.only	Molality 8.31852E-01 9.99622E+00 5.60950E+00 5.79856E-04 2.09763E-04 2.09763E-04 2.09763E-05 3.72379E-07 2.58813E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	7.78030E-01 1.0000E+00 5.29073E+00 2.14695E-04 6.3904&E-04 1.01191E-04 9.68710E-09 1.01460E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29229E-05 1.76808E-05 3.9682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31681E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 1.87794E-04 4.55260E-05 3.33916E-07 1.3960E-07 1.27238E-08 1.4149E-10 2.70215E-10 1.62527E-14 3.36963E-16 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3537E-04 8.33180E-05 7.2966E-09 1.02121E-10 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00
40012044500445012004500012004500014204555550	Species Name H20 NaHpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(OH)2- NaD4(aq) NpO2(CO3)3==- NpO2(0H)2- Na2CO3.H20Na2 Na2CO3.H20NA2 NA2CO3.H20NA2	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(SO3)2=- NpO2(SO3)2=- Natron N	Molality 8.31852E-01 9.99622E+00 5.6103E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.75603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000	1.92999E+01 3.47550E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.6444E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.02225-04 1.87794E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.27238E-08 2.14149E-10 2.70215E-10 1.62527E-14 3.36963E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.33537E-04 3.93550E-02 2.16337E-04 3.93550E-02 2.16337E-04 3.93550E-02 2.16337E-04 3.93550E-02 1.0212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
40012044500445012004500012004500014204555550	Species Name H20 NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)3=- NpO2(O3)3=- NpO2(O3)3=- NpO2(O3)2.2H20_ Na2CO3.1DH20Na2 Na2CO3.1DH20NA2 Na2CO3.1DH20.1DH20 Na2CO3.1DH20 Na2CO3.1DH20 Na2CO3.1DH20 Na2CO3.1DH20 Na2CO3.1DH20 Na2CO3	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(SO3)2=- NpO2(SO3)2=- Natron N	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.60950E+00 5.79836E-04 2.09763E-04 5.08519E-05 3.7279E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00 0.0000E+0	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3637E-04 3.93550E-02 2.3626E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+
80012808979999000000000000000000000000000000	Species Name H20 NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)3=- NpO2(O3)3=- NpO2(O3)3=- NpO2(O3)2.2H20_ Na2CO3.1DH20Na2 Na2CO3.1DH20NA2 Na2CO3.1DH20.1DH20 Na2CO3.1DH20 Na2CO3.1DH20 Na2CO3.1DH20 Na2CO3.1DH20 Na2CO3.1DH20 Na2CO3	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2(aq) NpO2(ag) NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3=- Trona Thermonatrite 2CO3-Heptahydrate Matron Natron Natron Stalite DiSABLED_DISABLED tittate.base.only NpO2OH(aged) tittate.acid.only	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.60950E+00 5.79836E-04 2.09763E-04 5.08519E-05 3.7279E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00 0.0000E+0	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3637E-04 3.93550E-02 2.3626E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+
8011284498449886976988898888981128245678985555555555555555555555555555555555	Species Name H20 NaHpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2(CO3)2=- NpO2(CO3)2=- NpO2(OB)2- NpO2(OB)2- NaB(CO3)2.2H20Na2 Na2CO3.H20NA2 Na2CO3.H2	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2(aq) NpO2(ag) NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3=- Trona Thermonatrite 2CO3-Heptahydrate Matron Natron Natron Stalite DiSABLED_DISABLED tittate.base.only NpO2OH(aged) tittate.acid.only	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 1.33591E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3637E-04 3.93550E-02 2.3626E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+
800120000000000000000000000000000000000	Speciés Name H20 NaHpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2(CO3)2=- NpO2CO3- OH- NpO2(CO3)2=- NpO2(OH)2- NaB(CO3)2.2H20 Na2CO3.H20Na2 Na2CO3.H20NA2 Na2	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2(aq) NpO2(ag) NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3==- Natcon Natcon SABLED_DISABLED CISABLED_DISABLED CISABLED_DISABLED CISABLED_DISABLED CISABLED_DISABLED CISABLED_CO3(aged) Citrate.acid.only * 5.9936	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 1.33591E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3637E-04 3.93550E-02 2.3626E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+
#0012074801601200480011401404505012048000120048000114014045555555555555555555555555	Species Name H20 NaNpO2CO3(s) H20 Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O1)2- Na3H(CO3)2.2H20Na2 Na2CO3.1H20NA2 Na2CO3.1H20 Na2CO3.1H2	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- NpO2(CO3)3==- NpO2(CO3)3=- NpO3(CO3)3=- NpO3(CO3)3=- NpO3(Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 1.33591E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
4041000410970000000000000000000000000000	Species Name H20 NaNpO2CO3(s) Ne+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NaCO3- N	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(OH)2=- Trona Thermonatrite ECO3-Heptahydrate Natron NATron NATron NATRON 	Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 1.33591E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
8001200400000000000000000000000000000000	Species Name H20 NaNpO2CO3(s) H20 Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O1)2- Na3H(CO3)2.2H20Na2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- NpO2(CO3)3==- NpO2(CO3)3=- NpO3(CO3)3=- NpO3(CO3)3=- NpO3(Molality 8.31852E-01 9.99622E+00 5.61003E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72979E-07 1.33591E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
#0112074500000000000000000000000000000000000	Species Name H20 NaNpO2CO3(s) H4 HCO3- CO2(aq) NpO2+ CO3= H4 NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O1)2- Na3H(CO3)2.2H20Na2 Na2CO3.7H20Na2 Na2CO3.1OH20NA2 Na2CO3.1OH20_NA2 Na2CO3.1OH20NA2 Na2CO3.1OH20NA2 Na2CO	WATER NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2(CO3)2=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)2=- NpO2	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72795E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00 0.000E+00 0.0000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+0	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
4041203410001200400001499011110145617104001128241034100	Species Name H20 NaNpO2CO3(s) Ne+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- Na3NpO2(CO3)2[s]_E Na2CO3.H2ONa2 Na2CO3.H2ONa2 Na2CO3.H2ONa2 NaCO3Na2 NaCO3Na2 NaCO3Na2 NpO2OR(aged) NpO2OR(aged) NpO2OR(aged) NpO2OR(aged) NpO2OR(aged) NpO2CH(amor) NpO2OR(aged) NpO2CH(amor) NpO2CH(amor) NpO2OR(aged) NpO2CH(amor)_ NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NDCH(amor) NDCH(amor)_ NDC	WATER NANPO2CO3(s) Na+ Cl- HCO3- CO2(aq) NPO2+ CO3= H+ NPO2CO3- OH- NPO2(CO3)2=- NPO2(CO3)2=- NPO2(CO3)2=- Trona Thermonatrite CCO3-Heptahydrate Natron 	Molality 8.31852E-01 9.99622E+00 5.60950E+00 5.79856E-04 2.09763E-04 2.09763E-04 2.09763E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
8011201410404750900120048000149091120140547124004420742004450750900120044509112014054750504202120044209	Species Name H20 NaMpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NaO2(aq) NpO2(CO3)2=- NaO2(aq) NaCO3(aq) NaCO3(aq) NaCO3(aq) NaCO3(aq) NaCO3(aq) NaCO3(aq) NaCO3(aq) NaCO3(aq) NaCO4(aq) NpO2CH(aqc) DaGH(aq) NDO2CH(aqc) DGM(H+)] DSMotic Coefficient Equilibrium RH (%) Ionic Strength (m) Density, kg/m3 NOTES: - Water "m - Gas "mol	WATER NANPO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2(aq) NpO2(aq) NpO2(co3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3=- Trona Thermonatrite CO3-Heptahydrate Torna Thermonatrite CO3-Heptahydrate Nahcolite Nahcolite Natron 	Molality 8.31852E-01 9.99622E+00 5.60950E+00 5.79856E-04 2.09763E-04 2.09763E-04 2.09763E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
#001200400000000000000000000000000000000	Species Name H20 NaNpO2CO3(s) H20 Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O1)2- Na3H(CO3)2.2H20Na2 Na2CO3.7H20Na2 Na2CO3.7H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 NoTES: - Water "m - "Descrip"	WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- Np	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.60950E+00 5.79856E-04 2.09763E-04 2.09763E-04 2.58813E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
409142634458960020048080001499011140456170140967828242667880	Species Name H20 NaNpO2CO3(s) Ne+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- Na3NpO2(CO3)2[s]_U Na2CO3.H20NA2CO3.H20NA2CO3.H	WATER NANPO2CO3(s) Na+ Cl- HCO3- CO2(aq) NPO2+ CO3= H+ NPO2CO3- OH- NPO2(CO3)2=- NPO2(CO3)2=- NPO2(CO3)2=- Trona Trona Trona Trona Trona Trona Natron 	Molality 8.31852E-01 9.99622E+00 5.60950E+00 5.79856E-04 2.09763E-04 2.09763E-07 2.58813E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 <th>7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00</th> <th>0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000</th> <th>1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00</th> <th>4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00</th> <th>8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+</th>	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.72603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
8001200410001200120010000000000000000000	Species Name H20 NaNpO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NaO2(aq) NpO2(CO3)2=- NaO2(ag) NaO2(CO3)2(s)_U NaCO3(s)2(s)_U NaCO3(s)2(s)_U NaCO3(s)2(s)_U NaCO3(s)2(s)_U NaCO3(s)2(s)_U NaCO4(ag)to.t NpO2CH(aged) NaO2(CO3)2(s)_U NaO2(CO3)2(s)_U NaO2(CO3)2(s)_U NaO2(CO3)2(s)_U NaO2(CO3)2(s)_U NaO2(CO3)2(s)_U NaO2(A(aged) NDO2CH(aged) NDO2CH(aged) NDO2CH(aged) NDTES: - Water 'm - Gas 'mO1 - 'Descrip *dG/RT/1 *Saturat	WATER NANPO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2(aq) NpO2(aq) NpO2(co3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3=- Trona Thermonatrite CO3-Heptahydrate Torana Thermonatrite CO3-Heptahydrate Nahcolite Nahcolite Natron Nahcolite Natron 	Molality 8.31852E-01 9.99622E+00 5.6103E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72379E-07 2.58815E-07 1.42123E-08 2.39201E-10 3.01825E-10 1.81540E-14 3.76383E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 1.65870 fraction H20 in a rity' are gas par-	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.75603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00 1.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
4091200400000000000000000000000000000000	Species Name H20 NaNpO2CO3(s) H20 Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O1)2- Na3H(CO3)2.2H20Na2 Na2CO3.7H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 NoTES: - Water "m - Descrip * dG/RT/1 * Saturat * Colored to the second to the s	WATER NANPO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- Np	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72795E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.75603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00 1.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+06 1.15465E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.02212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+
8001200410001200120010000000000000000000	Species Name H20 NaNpO2CO3(s) H20 Na+ C1- HCO3- CO2(aq) NpO2+ CO3= H+ NpO2CO3- OH- NpO2(CO3)2=- NpO2(O3)2=- NpO2(O3)2=- NpO2(O1)2- Na3H(CO3)2.2H20Na2 Na2CO3.7H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 NoTES: - Water "m - Descrip * dG/RT/1 * Saturat * Colored to the second to the s	WATER NANPO2CO3(s) Na+ Cl- HCO3- CO2(aq) NpO2(aq) NpO2(aq) NpO2(co3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- NpO2(CO3)3==- NpO2(CO3)3=- Trona Thermonatrite CO3-Heptahydrate Torana Thermonatrite CO3-Heptahydrate Nahcolite Nahcolite Natron Nahcolite Natron 	Molality 8.31852E-01 9.99622E+00 5.61032E+00 5.60950E+00 5.79856E-04 2.09763E-04 5.08519E-05 3.72795E-07 1.33591E-07 1.42123E-08 2.39201E-10 3.01826E-10 1.81540E-14 3.76383E-16 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000	7.78030E-01 1.0000E+00 5.29080E+00 5.29073E+00 2.14695E-04 6.09044E-04 1.01191E-04 9.68710E-09 1.01480E-06 2.43057E-07 7.75603E-09 6.19248E-15 3.01826E-10 1.43698E-23 1.12471E-16 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00 1.0000E+00	0.9353 1.000 0.9431 0.9432 0.3703 2.903 1.990 2.5972E-02 3.921 1.819 0.5436 2.5888E-05 1.000 7.9155E-10 0.2988 1.000 1.	1.92999E+01 3.47560E+00 1.95037E+00 2.01611E-04 7.29329E-05 1.76808E-05 1.29682E-07 8.99871E-08 4.64484E-08 4.94149E-09 8.31683E-11 1.04942E-10 6.31199E-15 1.30865E-16 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96951E+01 6.94928E+00 5.02247E+00 5.0220E+00 5.19125E-04 4.55260E-05 3.33916E-07 2.31707E-07 1.9600E-07 1.7238E-08 2.14149E-10 2.70215E-10 0.6000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	8.95267E+05 3.15056E+05 1.78045E+05 3.16755E+01 8.26478E+00 1.22486E+01 2.00380E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3357E-04 3.93550E-02 2.3636E-09 1.0212E-10 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.00000E+00 0.000E+00 0.000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000E+00 0.000E+00

Osmotic Coefficient=

Equilibrium RH (%) =

Ionic Strength (m) =

62...

622

- . *i*

1.241601

77.805007

5.610057

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

833 Total G/RT= -4.63462770E+03 Flashing Titration # 530 # inversions for batch pblm 14 337 IBenchmark TITRATE Problem, LOG10 option; Np(V)02 with CO3 in 5.61molal NaCl FMT V2.0 DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-C1-C1O4 (NR94); 538 (1) 95.01.31 Am(III)-Na-C1-C03-S04-P04 (FRSR89, FRF90, P91, RFFR92, RFF94, RRFF94) 1.00000E+00 [=] ATM Temperature= 2.98E+02 [#] Kelvin 2.4.2 Pressure² 542 Elemental Abundances for Flash Problem ÷ć: Ag. Molality Ac. Molarity Aq. mg/liter Total Moles 56. 0.40 1.00176739E+05 Hydrogen 1.11018357E+02 9.93915462E+01 3.86060470E+01 3.66820273E+01 5.55118409E+01 4.96981566E+01 7 95140687E+05 Oxygen 1.15465478E+05 5 42646354E+00 543 5 61000023E+00 5.02247206E+00 Sodium 0.0000000E+00 0.0000000E+00 0.0000000E+00 Potassium 541 0.0000000E+00 0.0000000E+00 0.0000000E+00 Magnesium 55.) 0.00000000E+00 0.0000000E+00 14 0.0000000E+00 0.00000000E+00 0.0000000E+00 Calcium 5.60889282E+00 5.02148063E+00 1.78026553E+05 Chlorine 1 95046284E+00 0.0000000E+00 0.0000000E+00 0 000000005+00 Sulfur 50% 0.0000000E+00 1.13304772E+01 564 580 9.43341702E-04 Carbon 3.47598202E+00 1.05369370E-03 0.0000000E+00 0.0000000E+00 0.0000000E+00 Posion 0.00000002+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 Neglon 0.0000000E+00 · • · · 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Air 0.0000000E+00 0.0000000E+00 0.0000000E+00 Boron 555 0.00000002+00 509 507 507 00000000E+00 0.0000000005+00 Bromine 0.00000000E+00 ٥ 0.0000000E+00 0.0000000E+00 TracerEl 0.000000005+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Th(IV) 56.3 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Am(III) 0.0000000E+00 0.0000000E+00 ${\mathcal C}_{i,j}$ 0.000000000000+00 0.0000000E+00 U(VI) 5.04731450E-07 4.51871569E-07 1.07115342E-01 Np(V)i.e.a 3.47561578E+00 .00000000E+00 0.00000000E+00 0.0000000E+00 C104+(EL) 3.07 0.0000000E+00 0 0.0000000E+00 0.00000000E+00 Phosphorus 880 0.0000000E+00 0 0000000E+00 5C7 0.0000000E+00 0.0000000E+00 0.0000000E+00 Electron 0.0000000E+00 -8.05334972E-16 -2.31587983E-15 -2.07334069E-15 0.0000000E+00 55 Charge 25.7 $\langle T \rangle$ Solution Parameters, Calculated 5.7 SOLUTION MASS 461.766388131816 grams 872 H20 MASS 347.744715353115 grams g/kgH20 873 572 TDS(g/kg) 327.889016696973 Specified Solution Density 675 675 1188.82089442743 $k\sigma/m^3 = \sigma/1$ DENSITY .7. Solution Parameters Based on Specified Density 373 0.388423849459858 578 SOLUTION VOL liters 560 293,549618380179 a/1 \sim 1188.82089442743 Density based on TDS and NaCl solutions g/1 5.2 533 Percent relative error vs NaCl density 0.000000000000000E+000 % 7.0% 525 -12: 21.1 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM 285 Molality Activity Act Coef Total Moles Molarity 509 Species Name 50 WATER 8.31857E-01 7.78050E-01 0.9353 1.93029E+01 4.96953E+01 H20 9.99473E+00 1.00000E+00 1 000 3 47562E+00 8.94800E+00 692 NaNpO2CO3(s)_ NaNp02C03(s) 5.29000E+00 1.95085£+00 5.02247E+00 0.9430 ÷43 Na+ Na+ 5.61000E+00 C1-5.60889E+00 5.28999E+00 0.9431 1.950462+00 5.02148E+00 . 4.0 C1-596 HCO3-HCO3-9.92660E-04 3.675438-04 0.3703 3.45192E-04 8 88700E-04 1.97480E-05 5.08414E-05 1.474942-06 2.5972E-02 500 CD3= CO3 = 5.67888E-05 1.17227E-05 1.40400E-06 3.61461E-06 CO2 (aq) 4.03745E-06 2.903 607 CO2 (ag) он-1.26397E-06 6.87170E-07 0.5437 4.39540E-07 1.13160E-06 328 он-2.991118-07 1.16182E-07 6.64703E-07 1.990 693 Np02+ NpO2+ 3.34101E-07 Np02C03-4.64631E-08 1.19620E-07 1.33613E-07 2.43094E-07 1.819 600 Np02C03-: US Np02 (C03)2=-Np02 (C03) 2=-3.64205E-08 9.43001E-13 2.5892E-05 1.26650E-08 3.26062E-08 1.01216E-09 2.60582E-09 2.91065E-09 1.14100E-08 3.920 602 H+ н+ Np02 (C03) 3==-3.33181E-19 7.9204E-10 1.46282E-10 3.76605E-10 303 Np02 (CO3) 3==-4.20660E-10 Np020H (ag) in. Np020H(aq) 1.76339E-10 1 76339E~10 1.000 6.13211E-11 1.57872E-10 6.80128E-15 1.75100E-14 5.84438E-15 0.2988 6:00 NpO2 (OH) 2-No02 (OH) 2-1.95583E-14 1.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.000 Na3H(CO3)2.2H20 Trona €ŬŠ 0.00000E+00 0.00000E+00 1 000002+00 1.000 0.00000E+00 07 Na2CO3 .H20____ _____Na2CO3-Heptahydrate 1.00000E+00 0.00000E+00 0.00000E+00 802 Na2CO3.7H2O 0.00000E+00 1.000 -909 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 Na2CO3.10H2O __Natron 610 Nahcolite 0 000002+00 1 00000E+00 1.000 0.00000E+00 0.00000E+00 NaHCO3 1.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.000 011 NaC1 Halite cú Na3Np02(CO3)2(s)_DISABLED_DISABLED 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 NaOH(aq).....to.titrate.base.only 0.00000E+00 0.00000E+00 0.000002+00 1 000 0 0000E+00 £13 0.00000E+00 0.00000E+00 NpO2OH (amor) 1.00000E+00 1.000 NpO2OH (amor) 0.00000E+00 3:4 1.00000E+00 1.000 0.00000E+00 0.00000E+00 NpO2OH (aged) 0.00000E+00 611 NpO2OH (aged) HCl(ag).....to.titrate.acid.only 0.00000E+00 6.5 0.00000E+00 0.00000E+00 1.000 0.00000E+00 618 pmH = -log[m(H+)]8.5360 £19 pH = -log(a(H+))= 7.9427



mg/liter

8.95271E+05

3.15011E+06

1.15465E+05

1.78027E+05

5.42259E+01

3.05095E+00

1.59078E-01

1.92454E-02

8.04750E-02

3.93616E-02

1.26859E-02

2.62641E-06

1.69124E-04

4.51598E-05

5.30660E-09

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.0000E+00

0.00000E+00

Descriptor

-4.23E-08

-9.18E-08

1.79E-07

3.21E-13

-1.15E-07

1.26E-07

-2.16E-07

-2.06E-08

-1.50E-07

-6.27E+00

~4.98E+00

-4.69E+00

-4.65E+00

-2.31E+00

-1.23E-01

-9.33E+02

-2.96E+02

-3.62E+00

-3.03E+00

-2.47E+02

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

...

C23 Density, kg/m3	= 1188.82							
<								
	molality is mole f							
	lality and activi ptor means:	ty are gas par	tiai pressures					
	ln10 for species wi	th nonzero conc.	s. (convergenc	e criterion)				
	tion Index for mine							
	activity) for aqueo			ncentrations				
	partial pressure) f	or gases						
-322								
	.63497997E+03							
5.5 Flashing Titratio 5.5 # inversions for		16						
(>> 1Benchmark TITRATE			th CO3 in 5.61	molal NaCl	FMT V2.0			
	FW86; Np(V)-Na-CO3-							
988 95.01.31 Am(III			P91, RFFR92, RFF	94, RRFF94)				
oca Pressure*	1.00000E+00 [=] AT	M Temperatu	re= 2.98E+	02 [=] Kelvin				
AC)	for Tlash Bushl							
(** Elemental Abundan (*)	ces for Flash Probl							
Total Moles	Aq. Molality	Aq. Molarity	Ag. mg/liter					
214		• •						
545 3.86146891E+01	1.11018383E+02	9.93917155E+01	1.00176910E+	05 Hydrogen				
6d* 3.66868155E+01		4.96994430E+01	7.95161268E+					
5.42690025£+00		5.02248064E+00	1.15465675E+					
0.00000000000000000000000000000000000		0.00000002+00 0.00000002+00	0.00000000E+ 0.00000000E+					
600 0.0000000E+00		0.00000000E+00	0.0000000E+					
		5.02068795E+00	1.77998450E+		•			
652 0.0000000E+00		0.0000000E+00	0.00000000E+					
3.47613771E+00		1.34388050E-03	1.61413487E+					
0.0000000E+00		0.0000000E+00	0.00000000E+					
CCC D.0000000E+00 SUC D.0000000E+00		0.00000000E+00	0.00000000E+ 0.00000000E+					
-55° 0.00000000E+00		0.0000000E+00	0.00000000E+					
ASE 0.0000000E+00		0.0000000E+00	0.0000000E+					
(%) 0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+	00 TracerEl				
C→> 0.0000000E+00		0.0000000E+00	0.00000000E+					
CO: 0.00000000000000000000000000000000000		0.00000000E+00 0.00000000E+00	0.00000000E+					
CO2 0.0000000E+00 603 3.47561578E+00		4.64127943E-07	1.10020694E-					
54- 0.00000000E+00		0.0000000E+00	0.00000000E+					
 Ess 0.0000000E+00		0.000000002+00		00 Phosphoru	s			
ීත් 0.0000000 E+0 0		0.0000000E+00	0.0000000E+					
	-2.95636061E-15 -	2.64674862E-15	0.00000000E+	00 Charge				
				po charge				
dif 100 Follopies Bourse	and Calculated			po chilige				
553 Solution Parame	ters, Calculated 461.86806085617	5 grams		po charge				
	ters, Calculated 461.86806085617 347.82247866665	•						
553 Solution Parame 170 SOLUTION MASS CT1 H20 MASS CT2 TDS (g/kg)	461.86806085617	1 grams						
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 TDS(g/kg) 173 273	461.86806085617 347.82247866665 327.88445021353	1 grams						
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 TDS(g/kg) 173 100 174 Specified Solut.	461.86806085617 347.82247866665 327.88445021353 ion Density	l grams 8 g/kgH2O						
553 Solution Parame 170 SOLUTION MASS 071 H20 MASS 073 H20 MASS 074 TDS (g/kg) 075 Specified Solution 074 DENSITY	461.86806085617 347.82247866665 327.88445021353	1 grams 8 g/kgH2O						
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 173 H20 MASS 174 TDS(g/kg) 175 974 175 DENSITY 176	461.86806085617 347.82247866665 327.88445021353 ion Density	1 grams 8 g/kgH2O 0 kg/m^3 =						
553 Solution Parame 170 SOLUTION MASS 071 H20 MASS 073 TDS(g/kg) 074 Specified Solut. 075 DENSITY 076 SOLUTION Parame 077 SOLUTION VOL	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters						
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 173 H20 MASS 174 TDS(g/kg) 175 Specified Solut. 176 DENSITY 178 Solution Parame 177 Solution Parame 178 Solution Parame 179 Solution Parame	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters						- - -
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 173 H20 MASS 174 TDS(g/kg) 175 GP/4 175 DENSITY 176 SOLUTION VOL 177 SOLUTION VOL 178 TDS 179 SOLUTION VOL	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters 2 g/l	g/l				1. 	1 1 1
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 173 TDS(g/kg) 173 BENSITY 174 DENSITY 175 SOLUTION PARAME 175 SOLUTION PARAME 175 SOLUTION VOL 175 SOLUTION VOL 175 DENSITY 175 SOLUTION VOL 175 DENSITY	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters 2 g/l tions 1188.8:	g/l 1855435140	g/1				· · · · · · · · · · · · · · · · · · ·
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 173 TDS(g/kg) 173 BENSITY 174 DENSITY 175 SOLUTION PARAME 175 SOLUTION PARAME 175 SOLUTION VOL 175 SOLUTION VOL 175 DENSITY 175 SOLUTION VOL 175 DENSITY	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters 2 g/l tions 1188.8:	g/l	g/1				2 2 2 2
 Solution Parame Solution Parame Solution MASS TDS (g/kg) TDS (g/kg) TDS (g/kg) Provide Solution Parame Solution Parame	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters 2 g/l tions 1188.8:	g/l 1855435140	g/1				· · · · · · · · · · · · · · · · · · ·
553 Solution Parame SOLUTION MASS C71 H20 MASS C71 H20 MASS C73 TDS(g/kg) C73 Specified Solut. C73 Solution Parame C75 SOLUTION VOL C75 SOLUTION VOL C75 TDS S00 Density based of 663 Percent relativ C64 C03	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters 2 g/l sity 0.00000	g/l 1855435140	g/1				
 Solution Parame Solution Parame Solution MASS H20 MASS TDS (g/kg) TDS Specified Solut. Based of Solution Parame Solution Parame Percent Parame Percent relative Concentration Concentration Concentration 	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters 2 g/l sity 0.00000	g/l 1855435140	g/1				1
553 Solution Parame SOLUTION MASS C71 H20 MASS C71 H20 MASS C73 TDS(g/kg) C73 Specified Solut. C73 Solution Parame C75 SOLUTION VOL C75 SOLUTION VOL C75 TDS S00 Density based of 663 Percent relativ C64 C03	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den	1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters 2 g/l sity 0.00000	g/l 1855435140 2000000000E+004	g/1	Total Moles	Molarity	mg/liter	Descriptor
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 173 H20 MASS 174 DENSITY 175 (g/kg) 175 175 Solution Parame 175 SOLUTION VOL 177 Solution Parame 175 SOLUTION VOL 177 TDS 180 180 180 180 180 180 180 180 180 180	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den	<pre>1 grams 8 g/kgH2O 10 kg/m^3 = fied Density 10 liters 2 g/l 10 liters 1188.81 10 0.000000 10 STEM Molality</pre>	g/l 1855435140	g/l 0 % Act Coef		Molarity	mg/liter	Descriptor
 Solution Parame Solution Parame Solution MASS TDS (g/kg) TDS (g/kg) TDS (g/kg) DENSITY DENSITY Solution Parame Solution Parame Solution Parame Density based of Percent relative Density based of D	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER	<pre>1 grams 8 g/kgH2O 0 kg/m^3 = fied Density 0 liters 2 g/l tions l188.8: sity 0.000000 STEM Molality 8.31862E-01</pre>	g/1 1855435140 000000000E+00 Activity 7.78067E-01	g/1 0 % Act Coef 0.9353	1.93072E+01	4.96954E+01	8.95273E+05	Descriptor
553 Solution Parame 170 SOLUTION MASS 677 H20 MASS 678 TDS(g/kg) 677 DENSITY 678 DENSITY 677 Solution Parame 677 Solution Parame 677 Solution Parame 677 Solution Parame 678 DENSITY 679 Density based of 680 Percent relative 681 Percent relative 682 TABLE OF CONCENTR 683 Species Name 684 Species Name 685 Species Name 686 Species Name 687 Species Name	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER NaNpO2CO3(s)	1 grams 8 g/kgH2O 0 kg/m ³ = fied Density 0 liters 2 g/l tions 1188.8: sity 0.000000 STEM Molality 8.31862E-01 9.99250E+00	g/l 1855435140 2000000000E+00 Activity 7.78067E-01 1.0000E+00	g/1 0 % Act Coef 0.9353 1.000	1.93072E+01 3.47562E+00	4.96954E+01 8.94601E+00	8.95273E+05 3.14941E+06	Descriptor
<pre>533 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 M20 MASS 173 B20 MASS 174 Specified Solut. 175 SOLUTION VOL 175 SOLUTION VOL 175 SOLUTION VOL 176 TDS 177 SOLUTION VOL 176 TDS 178 Density based of 178 B20 Density based of 178 B</pre>	461.8506085617 347.8247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54595179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER NaMp02C03(s) Na+	1 grams 8 g/kgH2O 10 kg/m^3 = fied Density 10 liters 2 g/l 188.82 sity 0.00000 STEM Molality 8.31862E-01 9.99250E+00 5.61000E+00	g/l 1855435140 000000000E+00 Activity 7.78067E-01 1.0000E+00 5.28971E+00	g/l 0 % Act Coef 0.9353 1.000 0.9429	1.93072E+01 3.47562E+00 1.95128E+00	4.96954E+01 8.94601E+00 5.02248E+00	8.95273E+05 3.14941E+06 1.15466E+05	Descriptor
<pre>5% Solution Parame 1% Solution MASS 1% H20 MASS 1% TDS(g/kg) 1% 1% 1% DENSITY 1% 1% 1% 1% 1% 1% 1% 1% 1% 1% 1% 1% 1%</pre>	461.86806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER NAMPO2CO3(s) Na+ Cl-	1 grams 8 g/kgH2O 10 kg/m^3 = fied Density 10 liters 2 g/l 10 tions 1188.8 188.8 188.8 188.8 188.8 188.8 188.8 188.8 188.8 188.8 188.8 188.8 199250 5.0000400 5.608005+00 5.608005+00	g/l 1855435140 000000000E+000 Activity 7.78067E-01 1.0000E+00 5.28971E+00 5.2887E+00	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431	1.93072E+01 3.47562E+00 1.95128E+00 1.95059E+00	4.96954E+01 8.94601E+00 5.02248E+00 5.02069E+00	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05	Descriptor
<pre>533 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 M20 MASS 173 B20 MASS 174 Specified Solut. 175 SOLUTION VOL 175 SOLUTION VOL 175 SOLUTION VOL 176 TDS 177 SOLUTION VOL 176 TDS 178 Density based of 178 B20 Density based of 178 B</pre>	461.8506085617 347.8247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54595179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER NaMp02C03(s) Na+	1 grams 8 g/kgH2O 10 kg/m^3 = fied Density 10 liters 2 g/l 188.82 sity 0.00000 STEM Molality 8.31862E-01 9.99250E+00 5.61000E+00	g/l 1855435140 000000000E+00 Activity 7.78067E-01 1.0000E+00 5.28971E+00	g/l 0 % Act Coef 0.9353 1.000 0.9429	1.93072E+01 3.47562E+00 1.95128E+00	4.96954E+01 8.94601E+00 5.02248E+00	8.95273E+05 3.14941E+06 1.15466E+05	Descriptor
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 TDS(g/kg) 173 Specified Solut 174 DENSITY 175 SOLUTION VOL 176 SOLUTION VOL 177 SOLUTION VOL 178 SOLUTION VOL 179 SOLUTION VOL 170 SOLUTION VOL 176 SOLUTION VOL 177 SOLUTION VOL 178 SPECIES NAME 179 SPECIES NAME 179 H20 179 NAHPO2CO3(s) 179 OU2	461.85806085617 347.82247866665 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54595179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER NaNpO2C03(s) Na+ C1- HCO3- OH-	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 10 liters 2 g/l 100 liters 2 g/l 100 liters 2 sity 0.00000 STEM Molality 8.31862E-01 9.99250E+00 5.6100E+00 5.6100E+00 1.00903E-03 4.9071F-04 1.07447E-05	g/l 1855435140 00000000000000000000000000000000000	g/l 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437	1.93072E+01 3.47562E+00 1.95128E+00 1.95059E+00 3.50963E-04	4.96954E+01 8.94601E+00 5.02248E+00 5.02069E+00 9.03356E-04	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01	Descriptor
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 177 TDS(g/kg) 173 OPENITY 174 DENSITY 175 SOLUTION PARAME 176 DENSITY 178 DENSITY 178 SOLUTION VOL 179 SOLUTION VOL 179 DENSITY 178 SOLUTION VOL 179 SOLUTION VOL 179 DENSITY based or 180 Percent relative 181 Species Name 182 Species Name 183 Species Name 184 Species OS (S) 182 NaPO2CO3(S) 184 HCO3- 185 CO3= 184 HCO3- 185 CO2(aq)	461.86806085617 347.82247866655 347.82247866655 327.88845021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER NaNpO2CO3(s) Na+ C1- HCO3- CO3= OH- CC2(aq)	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 10 liters 2 g/l 11005 ll88.81 1188.82 1189.81 1199.81 119	g/l 1855435140 200000000000000000000000000000000000	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904	1.93072E+01 3.47562E+00 1.95128E+00 1.95059E+00 3.50963E-04 1.70682E-06 1.67895E-07	4.96954E+01 8.94601E+00 5.02248E+00 5.02069E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.90188E-02	-4.59E-08 -8.67E-08
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 H20 MASS 173 TDS(g/kg) 173 Specified Solut. 174 DENSITY 175 SOLUTION VOL 177 Solution Parame 177 Solution Parame 177 Solution Parame 178 SOLUTION VOL 179 TDS 180 Percent relativ 181 OF CONCENTR 182 Species Name 183 Species Name 184 Species Name 183 Species Name 184 Species Of (s) 192 NathO2CO3(s) 193 C1+ 194 C03+ 195 C04+ 197 C02(aq) 197 Np02(C03)2*-	461.8500605517 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER NaNp02C03(s) Na+ Cl- HC03- C03= OH- C02(aq) Np02(C03)2=-	1 grams 8 g/kgH2O 10 kg/m^3 = fied Density 10 liters 2 g/l 10 sity 0.00000 10 sity 10 sity 0.00000 10 sity 10	g/l 1855435140 00000000000000000000000000000000000	g/l 0 % Act Coef C.9353 l.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05	1.93072E+01 3.47562E+00 1.95128E+00 3.5059E+00 3.50963E-04 1.70682E-04 3.73726E-06 1.67895E-07 1.09415E-07	4.96954E+01 8.94601E+00 5.02248E+00 9.03356E-04 4.39325E-04 4.39325E-04 4.32150E-07 2.81627E-07	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E+01 1.90188E-02 1.09571E-01	-4.59E-08 -8.67E-08 2.59E-08
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 TDS(g/kg) 173 Specified Solut 174 DENSITY 175 SOLUTION VOL 176 SOLUTION VOL 177 SOLUTION VOL 178 SOLUTION VOL 179 SOLUTION VOL 176 SOLUTION VOL 177 SOLUTION VOL 178 SPECIES NAME 180 Species Name 181 Species Name 182 TABLE OF CONCENTR 183 Species Name 184 SOC 185 Species Name 186 CO3= 187 CO2(aq) 188 NPO2(CO3)2a-	461.8500605517 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54595179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER NaNp02C03(s) Na+ Cl- HCO3- OH- CC2(aq) Np02(C03)2=- Np02C03-	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 tions 1188.82 11 sity 0.00000 STEM Molality 8.31862E-01 9.99250E-00 5.6100E+00 1.0903E-03 4.9071E-04 1.07447E-05 4.82702E-07 3.14571E-07 1.33630E-07	g/l 1855435140 D0000000000E+000 Activity 7.78067E-01 1.0000E+00 5.28971E+00 5.28971E+00 5.28971E+00 5.28972E-04 1.274452-05 5.84190E-06 1.40153E-06 8.14859E-12 2.43107E-07	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819	1.93072E+01 3.47562E+00 1.95128E+00 1.95059E+00 3.50963E-04 1.70682E-04 3.73726E-06 1.67895E-07 1.09415E-07 4.64794E-08	4.96954±01 8.94601±+00 5.02248±+00 9.03356±-04 4.39325±-04 9.61946±-06 4.32150±-07 2.81627±-07 1.19635±-07	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.99188E-02 1.99573E-01 3.93666E-02	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 177 TDS(g/kg) 178 Specified Solut. 179 DENSITY 178 DENSITY 178 DENSITY 178 DENSITY 178 SOLUTION VOL 179 SOLUTION VOL 179 SOLUTION VOL 179 SOLUTION VOL 179 SOLUTION VOL 170 TDS 170 Percent relativ 171 TABLE OF CONCENTR 172 Species Name 173 Species Name 174 HC03- 175 CO2 174 HC03- 175 OH- 175 Np02(C03)2a- 170 Np02+	461.86806085617 347.82247866655 347.82247866655 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER NaNpO2CO3 (s) Na+ C1- HCO3- CO3= OH- C02(aq) NpO2(CO312=- NpO2(C) NpO2(C)	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 tions 1188.8: 1183.8:	g/l 1855435140 D000000000E+000 Activity 7.78067E-01 1.00000E+00 5.28871E+00 5.2887E+00 3.73572E-04 1.27445E-05 5.84190E-06 1.40153E-06 8.14859E-12 2.43107E-07 7.63314E-08	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.965	1.93072E+01 3.47562E+00 1.95128E+00 3.50963E-04 1.70682E-04 3.73726E-06 1.67895E-07 1.09415E-07 4.64794E-08 1.34540E-08	4.96954E+01 8.94601E+00 5.02248E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07 2.81627E-07 3.46298E-08	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 1.63601E-01 1.90188E-02 1.09571E-01 3.93666E-02 9.31704E-03	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 TDS(g/kg) 173 TDS(g/kg) 174 Specified Solut 175 DENSITY 178 DENSITY 178 SOLUTION VOL 179 SOLUTION VOL 170 TDS 170 SOLUTION VOL 171 TDS 172 TABLE OF CONCENTR 173 Species Name 174 SOL 175 SOL 176 NPO2CO3(s) 177 NPO2(CO3) 178 NPO2(CO3) 179 NPO2(CO3)	461.8500605517 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54595179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER NaNp02C03(s) Na+ Cl- HCO3- OH- CC2(aq) Np02(C03)2=- Np02C03-	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 tions 1188.82 11 sity 0.00000 STEM Molality 8.31862E-01 9.99250E-00 5.6100E+00 1.0903E-03 4.9071E-04 1.07447E-05 4.82702E-07 3.14571E-07 1.33630E-07	g/l 1855435140 D0000000000E+000 Activity 7.78067E-01 1.0000E+00 5.28971E+00 5.28971E+00 5.28971E+00 5.28972E-04 1.274452-05 5.84190E-06 1.40153E-06 8.14859E-12 2.43107E-07	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819	1.93072E+01 3.47562E+00 1.95128E+00 3.50958E+00 1.70682E-04 3.73726E-06 1.67895E-07 1.09415E-07 4.64794E-08 1.34540E-08 1.05097E-08	4.96954+01 8.94601E+00 5.02248E+00 5.02059E+00 9.0335E-04 9.61946E-06 4.32150E-07 2.81627E-07 1.19635E-07 3.46298E-08 2.80808E-08	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.9018E-02 1.09571E-01 3.9366E+02 9.31704E-03 1.26104E-02	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08 4.49E-08
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 177 TDS(g/kg) 173 Specified Solut. 174 DENSITY 175 SOLUTION MASS 177 TDS(g/kg) 178 DENSITY 178 DENSITY 178 DENSITY 179 Solution Parame 175 SOLUTION VOL 177 Solution Parame 178 DENSITY 179 Solution Parame 170 Solution Parame 171 Solution Parame 172 Solution Parame 173 Percent relativ 174 TDS 175 Solution Parame 176 Percent relativ 177 TDS 178 Species Name 179 Parcent selativ 170 NaNp02C03(s) 171 Np02(C03)2z= 172 Np02(C03)3=== 173 <th>461.86806085617 347.82247866655 347.82247866655 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- H+ NpO2(CO3)3=- H+ NpO2(CO3)3=- H+</th> <th>1 grams 8 g/kgH2O 10 kg/m³ = fied Density 10 liters 2 g/l 11 sity 0.000000 12 sity 0.000000 13 sity 0.000000 14 sity 0.000000 15 sity 0.00000 15 sity 0.0000 15 sity 0.00000 15 sity 0.000000 15 sity 0.000000 15 sity 0.000000 15 sity 0.000000 15 sity 0.0000000 15 sity 0.000000 15 sity 0.0000000 15 sity 0.0000000 15 sity 0.000000000000 15 sity 0.00000000000000000000000000000000000</th> <th>g/l 1855435140 D00000000000000000000000000000000000</th> <th>g/l 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10</th> <th>1.93072E+01 3.47562E+00 1.95128E+00 3.50963E-04 1.70682E-04 3.73726E-06 1.67895E-07 1.09415E-07 4.64794E-08 1.34540E-08</th> <th>4.96954E+01 8.94601E+00 5.02248E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07 2.81627E-07 3.46298E-08</th> <th>8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 1.63601E-01 1.90188E-02 1.09571E-01 3.93666E-02 9.31704E-03</th> <th>-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08</th>	461.86806085617 347.82247866655 347.82247866655 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER NaNpO2CO3(s) Na+ C1- HCO3- CO2(aq) NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- H+ NpO2(CO3)3=- H+ NpO2(CO3)3=- H+	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 sity 0.000000 12 sity 0.000000 13 sity 0.000000 14 sity 0.000000 15 sity 0.00000 15 sity 0.0000 15 sity 0.00000 15 sity 0.000000 15 sity 0.000000 15 sity 0.000000 15 sity 0.000000 15 sity 0.0000000 15 sity 0.000000 15 sity 0.0000000 15 sity 0.0000000 15 sity 0.000000000000 15 sity 0.00000000000000000000000000000000000	g/l 1855435140 D00000000000000000000000000000000000	g/l 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10	1.93072E+01 3.47562E+00 1.95128E+00 3.50963E-04 1.70682E-04 3.73726E-06 1.67895E-07 1.09415E-07 4.64794E-08 1.34540E-08	4.96954E+01 8.94601E+00 5.02248E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07 2.81627E-07 3.46298E-08	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 1.63601E-01 1.90188E-02 1.09571E-01 3.93666E-02 9.31704E-03	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 TDS(g/kg) 173 GP/4 174 Specified Solut. 175 GP/4 174 DENSITY 177 Solution Parame 177 Solution Parame 177 Solution Parame 177 Solution Parame 178 Solution Parame 179 Solution Parame 179 Solution Parame 179 Solution Parame 170 Post 170 Post 171 Solution Parame 172 Solution Parame 173 Solution Parame 174 Post 175 Solution Parame 176 Post 177 Solution Parame 178 Post 179 Nol 170 Npo2(co3)(s) 171 Npo2(co3) 3==- 172	461.86806085617 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER NaNpO2CO3(s) Na+ Cl- HCO3- CO3= OH- CC2(aq) NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- H+ NpO2(CO3)3=- H+ NpO2(CO3)2=- NpO2(CO3)2=- H+ NpO2(CO3)2=- N	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 sity 0.00000 12 sity 0.00000 13 sity 0.00000 14 sity 0.00000 15 sity 0.00000 15 sity 0.00000 16 sity 0.0000 16 sity 0.0000 17 sity 0.0000 16 sity 0.0000 16 sity 0.0000 16 sity 0.0000 17 sity 0.0000 16 sity 0.0000 17 sity 0.0000 17 sity 0.0000 16 sity 0.0000 16 sity 0.0000 17 sity 0.00000 17 sity 0.00000 17 sity 0.00000 17 sity 0.00000 17 sity 0.00000 17 sity 0.00000 17 sity 0.000000 17 sity 0.000000 17 sity 0.00000000 17 sity 0.00000000000 17 sity 0.00000000000000000000000000000000000	g/l 1855435140 D00000000000000000000000000000000000	g/l 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10 3.919 1.000 0.2988	1.93072E+01 3.47562E+00 1.95128E+00 1.5059E+00 3.50952E-04 3.73726E-06 1.67895E-07 4.64794E-08 1.34540E-08 1.99415E-07 4.64794E-08 1.39134E-10 6.03495E-11 5.69085E-14	4.96954+01 8.94601E+00 5.02248E+00 5.02059E+00 9.0335E=04 9.61946E=06 4.32150E-07 2.81627E-07 1.19635E=07 3.46298E=08 3.06642E=10 1.55336E=10 1.46479E=13	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.9018E=02 1.09571E-01 3.93666E+02 9.31704E+03 1.26104E+02 3.09064E+07 4.44344E+05 4.43921E+08	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08 4.49E-08 ~2.55E-08 4.70E-09 2.99E-08
<pre>533 Solution Parame 170 SOLUTION MASS 171 H20 MASS 173 TDS(g/kg) 173 1725(g/kg) 173 1742 MASS 174 175 175 175 177 Solution Parame 175 SOLUTION VOL 175 175 175 175 175 175 175 175 175 175</pre>	461.8500605617 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER MANDO2CO3(s) Na+ Cl- HCO3- CO3= OH- CO3= OH- CO2(aq) NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- H+ NpO2(Haq) NpO2(OH)2- Trona	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 tions 1188.8: 12 sity 0.00000 13 tions 1188.8: 18 sity 0.00000 18 tions 1188.8: 18 sity 0.00000 19 92502-01 5.60800E+00 5.60800E+00 1.07447E-05 4.82702E-07 3.1457E-07 1.3630E-07 3.86807E-08 3.13656E-08 3.1365E-08 3.1365E-08 3.1355E-08 3.1355E-10 1.7357E-10 1.63614E-13 0.0000E+00	g/l 1855435140 200000000000000000000000000000000000	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10 3.919 1.000 0.2988 1.000	1.93072E+01 3.47562E+00 1.95128E+00 3.50961E-04 3.73726E-06 1.67895E-07 1.9415E-07 4.64794E-08 1.34540E-08 1.9937E-08 1.9134E-10 6.03495E-11 5.69085E-14 0.00000E+00	4.96954E+01 8.94601E+00 5.02248E+00 9.03356E-04 4.39325E-04 9.61946E-05 4.32150E-07 2.81627E-07 1.19635E-07 3.46298E-08 3.06642E-10 1.55336E-10 1.46479E-13 0.00000E+00	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.99188E-02 1.99571E-01 3.93666E-02 9.31704E-03 3.09064E-07 4.44344E-05 4.43921E-08 0.00000E+00	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08 4.49E-08 ~2.55E-08 4.70E-09 2.99E-08 -5.33E+00
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 173 TDS(g/kg) 173 Specified Solut. 174 DENSITY 175 SOLUTION MASS 177 TDS(g/kg) 178 DENSITY 179 Solution Parame 175 SOLUTION VOL 177 Solution Parame 178 Solution Parame 179 Solution Parame 170 Solution Parame 175 Solution Parame 176 Solution Parame 177 Solution Parame 178 Nale 179 Nale 170 Nale	461.86806085617 347.82247866655 347.82247866655 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER WATER NaNpO2CO3 (s) Na+ C1- HCO3- CO3= OH- C02(aq) NpO2(CO3)2=- NpO2(CO3)3=- H+ NpO2(CO3)3=- H+ NpO2(CO3)3=- H- NpO2(CO3)3=- H+ NpO2(CO3)3=- Trona Thermonatrite	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 tions 1188.8 1.0000 1.0000 1.000 1.3630 1.3656 1.000 1.3636 1.3656 1.000 1.3636 1.3656 1.000 1.3636 1.3656 1.000 1.3636 1.3656 1.000 1.3636 1.3656 1.000 1.63614 1.13 0.0000 1.0000 1.00000 1.00000 1.00000 1.00000 1.00000 1.0000	g/l 1855435140 D000000000E+000 Activity 7.78067E-01 1.0000E+000 5.28871E+00 3.73572E-04 1.27445E-05 5.84190E-06 1.40153E-06 8.14859E-12 2.43107E-07 7.69314E-08 2.48770E-17 1.34216E-09 1.73507E-10 4.88873E-14 1.00002E+00 1.00002E+00	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10 3.919 1.000 0.2988 1.000	1.93072E+01 3.47562E+00 1.95128E+00 1.95059E+00 3.50963E-04 1.70682E-04 3.73726E-06 1.6785E-07 1.99415E-07 4.64794E-08 1.34540E-08 1.34540E-08 1.34540E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9907	4.96954E+01 8.94601E+00 5.02248E+00 5.02059E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07 1.19635E-07 3.46298E-08 3.06642E-10 1.55336E-10 1.46479E-13 0.00000E+00	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.99188E-02 9.31704E-03 3.93666E+02 9.31704E-03 1.26104E-02 3.93064E+07 4.44344E+05 4.43921E+08 0.00000E+00	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08 4.49E-08 -2.55E-08 4.70E-09 2.99E-08 5.33E+00 -4.042+00
553 Solution Parame 170 SOLUTION MASS 171 H20 MASS 172 TDS(g/kg) 173 Specified Solut. 174 DENSITY 175 SOLUTION VOL 177 SOLUTION VOL 178 SOLUTION VOL 179 SOLUTION VOL 170 POC 171 TDS 172 TABLE OF CONCENTR 173 Species Name 170 NPO2CO3 (s)	461.86806085617 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER MaNpO2CC03(s) Na+ Cl- HCO3- CO3= OH- CC2(aq) NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- H+ NpO2(CO3)3=- H+ NpO2(CO3)3=- H+ NpO2(CO3)2=- Thermonatrite 2CO3-Heptahydrate	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 sity 0.000000 12 sity 0.000000 13 sity 0.000000 14 sity 0.000000 14 sity 0.00000 14 sity 0.0000 14 sity 0.0000 14 sity 0.0000 14 sity 0.000 15 sity 0.0000 15 sity 0.00000 15 sity 0.00000 15 sity 0.00000 15 sity 0.00000 15 sity 0.0000000 15 sity 0.000000 15 sity 0.0	g/l 1855435140 D00000000000000000000000000000000000	g/l 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10 3.919 1.000 0.2988 1.000 1.000	1.93072E+01 3.47562E+00 1.95128E+00 1.5059E+00 3.50952E-04 3.73726E-06 1.67895E-07 4.64794E-08 1.34540E-08 1.93947E-08 1.9134E-10 6.03495E-11 5.69085E-14 0.0000E+00 0.0000E+00	4.96954+01 8.94601E+00 5.02248E+00 5.02059E+00 9.0335E-04 9.61946E-06 4.32150E-07 2.81627E-07 1.19635E-07 2.81627E-07 3.46298E0 8.0808E-08 3.06642E-10 1.55336E-10 1.6479E-13 0.00000E+00 0.00000E+00	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.9018E-02 1.09571E-01 3.93666E+02 9.31704E+03 1.26104E+02 3.09064E+07 4.44344E+05 4.43921E+08 0.00000E+00 0.00000E+00	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -1.12E-08 4.49E-08 -2.55E-08 4.70E-09 2.99E-08 -5.33E+00 -4.042E+00 -3.75E+00
553 Solution Parame 170 SOLUTION MASS 171 TDS(g/kg) 173 TDS(g/kg) 174 DENSITY 175 Solution Parame 175 Solution Parame 176 DENSITY 177 Solution Parame 175 Solution Parame 176 DENSITY 178 Solution Parame 179 Solution Parame 175 Solution Parame 176 Density based or 178 Density based or 179 Parcent relative 170 Species Name 171 Species Name 172 NaNpO2CO3(s) 173 NaPO2CO3(s) 174 NPO2(CO3)2= 175 NpO2(C03)2= 176 Na2CO3.102 178 Na2CO3.11042 179 Na2CO3.11042 174 Na2CO3.11042	461.86806085617 347.82247866655 347.82247866655 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER WATER NaNpO2CO3 (s) Na+ C1- HCO3- CO3= OH- C02(aq) NpO2(CO3)2=- NpO2(CO3)3=- H+ NpO2(CO3)3=- H+ NpO2(CO3)3=- H- NpO2(CO3)3=- H+ NpO2(CO3)3=- Trona Thermonatrite	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 tions 1188.8 1.0000 1.0000 1.000 1.3630 1.3656 1.000 1.3636 1.3656 1.000 1.3636 1.3656 1.000 1.3636 1.3656 1.000 1.3636 1.3656 1.000 1.3636 1.3656 1.000 1.63614 1.13 0.0000 1.0000 1.00000 1.00000 1.00000 1.00000 1.00000 1.0000	g/l 1855435140 D000000000E+000 Activity 7.78067E-01 1.0000E+000 5.28871E+00 3.73572E-04 1.27445E-05 5.84190E-06 1.40153E-06 8.14859E-12 2.43107E-07 7.69314E-08 2.48770E-17 1.34216E-09 1.73507E-10 4.88873E-14 1.00002E+00 1.00002E+00	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10 3.919 1.000 0.2988 1.000	1.93072E+01 3.47562E+00 1.95128E+00 1.95059E+00 3.50963E-04 1.70682E-04 3.73726E-06 1.6785E-07 1.99415E-07 4.64794E-08 1.34540E-08 1.34540E-08 1.34540E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9917E-08 1.9907	4.96954E+01 8.94601E+00 5.02248E+00 5.02059E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07 1.19635E-07 3.46298E-08 3.06642E-10 1.55336E-10 1.46479E-13 0.00000E+00	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.99188E-02 9.31704E-03 3.93666E+02 9.31704E-03 1.26104E-02 3.93064E+07 4.44344E+05 4.43921E+08 0.00000E+00	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08 4.49E-08 -2.55E-08 4.70E-09 2.99E-08 5.33E+00 -4.042+00
553 Solution Parame 170 SOLUTION MASS 171 TDS(g/kg) 173 TDS(g/kg) 174 DENSITY 175 Solution Parame 174 DENSITY 175 Solution Parame 176 DENSITY 177 Solution Parame 177 Solution Parame 178 DENSITY 179 Solution Parame 177 Solution Parame 178 DENSITY 178 Solution Parame 179 Solution Parame 170 TDS 177 Solution Parame 178 Density based on 179 Parcent relative 170 TABLE OF CONCENTR 170 TAD 170 TAD 170 Nato 170 Nato 171 Nato 172 Nato 173 Nato 174 Nato <t< th=""><th>461.86806085617 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER MANPO2CO3(s) Na+ Cl- HCO3- CO3= OH- CC2(aq) NpO2(CO3)2=- NpO2CO3- NpO2(CO3)2=- H+ NpO2(CO3)3=- H+ NpO2(CO3)3=- H+ NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- H+ NpO2(CO3)2=- H- NpO2(CO3)2=- NpO3(NpO3)2=- NpO3(NpO3)2=- NpO3(NpO3)2=- NpO3(NpO3)2=- NpO3(NpO3)2</th><th>1 grams 8 g/kgH2O 10 kg/m³ = fied Density 10 liters 2 g/l 11 ters 2 g/l 12 tions 1188.81 18</th><th>g/l 1855435140 D00000000000000000000000000000000000</th><th>g/l 0 % Act Coef C.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10 3.919 1.000 0.2988 1.000 1.000 1.000</th><th>1.93072E+01 3.47562E+00 1.95128E+00 1.5059E+00 3.50952E-04 3.73726E-06 1.09415E-07 4.64794E-08 1.34540E-08 1.34540E-08 1.9134E-10 6.03495E-11 5.69085E-14 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00</th><th>4.96954+01 8.94601E+00 5.02248E+00 5.02059E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07 2.81627E-07 1.19635E-07 3.46298E-08 3.06642E-10 1.55336E-10 1.46479E-13 0.0000E+00 0.00000E+00 0.00000E+00</th><th>8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.9018E-02 1.09571E-01 3.9366E+02 3.9366E+02 3.9366E+02 3.93064E+07 4.44344E+05 4.43921E-08 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00</th><th>-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 2.13E-08 4.49E-08 ~2.55E-08 4.70E-09 2.99E-08 -5.33E+00 -3.75E+00 -3.75E+00 -3.75E+00 -2.30E+00 +1.24E-01</th></t<>	461.86806085617 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER MANPO2CO3(s) Na+ Cl- HCO3- CO3= OH- CC2(aq) NpO2(CO3)2=- NpO2CO3- NpO2(CO3)2=- H+ NpO2(CO3)3=- H+ NpO2(CO3)3=- H+ NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- H+ NpO2(CO3)2=- H- NpO2(CO3)2=- NpO3(NpO3)2=- NpO3(NpO3)2=- NpO3(NpO3)2=- NpO3(NpO3)2=- NpO3(NpO3)2	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 ters 2 g/l 12 tions 1188.81 18	g/l 1855435140 D00000000000000000000000000000000000	g/l 0 % Act Coef C.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10 3.919 1.000 0.2988 1.000 1.000 1.000	1.93072E+01 3.47562E+00 1.95128E+00 1.5059E+00 3.50952E-04 3.73726E-06 1.09415E-07 4.64794E-08 1.34540E-08 1.34540E-08 1.9134E-10 6.03495E-11 5.69085E-14 0.0000E+00 0.0000E+00 0.00000E+00 0.0000E+00	4.96954+01 8.94601E+00 5.02248E+00 5.02059E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07 2.81627E-07 1.19635E-07 3.46298E-08 3.06642E-10 1.55336E-10 1.46479E-13 0.0000E+00 0.00000E+00 0.00000E+00	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.9018E-02 1.09571E-01 3.9366E+02 3.9366E+02 3.9366E+02 3.93064E+07 4.44344E+05 4.43921E-08 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 2.13E-08 4.49E-08 ~2.55E-08 4.70E-09 2.99E-08 -5.33E+00 -3.75E+00 -3.75E+00 -3.75E+00 -2.30E+00 +1.24E-01
553 Solution Parame 170 SOLUTION MASS 171 TDS(g/kg) 173 TDS(g/kg) 174 DENSITY 175 Solution Parame 175 Solution Parame 176 DENSITY 177 Solution Parame 175 Solution Parame 176 DENSITY 178 Solution Parame 179 Solution Parame 175 Solution Parame 176 Density based or 178 Density based or 179 Parcent relative 170 Species Name 171 Species Name 172 NaNpO2CO3(s) 173 NaPO2CO3(s) 174 NPO2(CO3)2= 175 NpO2(C03)2= 176 Na2CO3.102 178 Na2CO3.11042 179 Na2CO3.11042 174 Na2CO3.11042	461.8500605617 347.82247866655 327.88445021353 ion Density 1188.8185543514 ters Based on Speci 0.38851013820874 293.54596179997 n TDS and NaCl solu e error vs NaCl den ATIONS FOR BATCH SY WATER WATER NaNp02C03(s) Na+ Cl- HC03- C03= 0H- C02(aq) Np02(C03)2=- Np02(C03)3=- H+ Np02(C03)3=- H+ Np02(C03)3=- H+ Np02(C03)2=- Np02(C	1 grams 8 g/kgH2O 10 kg/m ³ = fied Density 10 liters 2 g/l 11 tions 1188.8 199.9 100002+00 1.00002+00 0.00002+00	g/l 1855435140 D00000000000000000000000000000000000	g/1 0 % Act Coef 0.9353 1.000 0.9429 0.9431 0.3702 2.5971E-02 0.5437 2.904 2.5904E-05 1.819 1.989 7.9313E-10 3.319 1.000 0.2988 1.000 0.2988 1.000 1.000 1.000	1.93072E+01 3.47562E+00 1.95128E+00 1.95059E+00 3.50961E-04 3.73726E-06 1.67895E-07 4.64794E-08 1.34540E-08 1.34540E-08 1.39134E-10 6.03495E-11 5.69085E-11 5.69085E-12 0.00000E+00 0.00000E+00 0.00000E+00	4.96954E+01 8.94601E+00 5.02248E+00 9.03356E-04 4.39325E-04 9.61946E-06 4.32150E-07 3.46298E-08 3.06642E-10 1.55336E-10 1.46479E-13 0.00000E+00 0.00000E+00 0.00000E+00	8.95273E+05 3.14941E+06 1.15466E+05 1.77998E+05 5.51202E+01 2.63636E+01 1.63601E-01 1.9371E-01 3.93666E-02 9.31704E-03 3.03064E-07 4.44344E-05 4.43921E-08 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	-4.59E-08 -8.67E-08 2.59E-08 4.47E-12 -2.13E-08 4.49E-08 ~2.55E-08 4.70E-09 2.99E-08 -5.33E+00 -4.042+00 -3.75E+00 -3.75E+00 -2.30E+00

Appendix N: Sample Output File "Np_NaCl BM LOG.OUT"

Np020H(ag)

1.71249E-10

1.71249E-10

1.000

5.95833E-11

1.53315E-10

4.38564E-05

1.06E~08

213 MpO2OH (amor) NoO2OH(amor) 0.00000E+00 1 000002+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.63E+00 Np020H(aged) 0.00000E+00 NoO2OH (aged) 1.00000E+00 1.000 0.000002+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 pinH = -log[m(H+)]9.4653 ֥, pH = -log[A(H+1] 8 8727 1.241539 Osmotic Coefficient= Equilibrium RH (%) = 77.806749 1 5.610494 77) 722 Ionic Strength (m) = 1188.82 Density, kg/m3 = 22. NOTES: - Water "molality" is mole fraction H2O in aqueous phase - Gas "molality" and "activity" are gas partial pressures 20 25 means: - "Descriptor" *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 -4,63548129£+03 Total G/RT= Flashing Titration # 6 # inversions for batch pblm 17 ?2: IBenchmark TITRATE Problem, LOGIO option; Np(V)02 with CO3 in 5.61molal NaCl FMT V2.0 (5) DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-C1-Cl04 (NR94); 232 95.01.31 Am(III)-Na-C1-C03-S04-P04 (FRSR89, FRF90, P91, RFFR92, RFF94, RRFF94) 1.5. Presenter 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin 706) 241 Elemental Abundances for Flash Problem 70 • ē] Total Moles Aq. Molality Aq. Molarity Ag. mg/liter 2.22 1.54 3.86270051E+01 9,93919460E+01 1.00177142E+05 Hydrogen 1.11018410E+02 245 245 5.55151239E+01 3.66936391E+01 4.97012721E+01 7.95190533E+05 Oxygen Sodium 5.42752260E+00 5.61000344E+00 5.02249276E+00 1.15465953E+05 267 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000000000 Potassium ter 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Magnesium وتهاز 0.0000000E+00 0.0000000E+00 0.000000000. 0.00000000E+00 Calcium 150 762 762 769 769 5.60672579E+00 1.95076678E+00 5.01955836E+00 1.77958403E+05 Chlorine 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Sulfur 3.47635958E+00 2.13880634E-03 1.91481868E-03 2.29988871E+01 Carbon 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Poston 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Neglon 0.00000005+00 0.0000000000000 0.0000000E+00 Air 75.4 76.7 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 Boron 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Bromine 763 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.0000000E+00 TracerEl 0.0000000E+00 752 0.0000000E+00 0.000000002+00 Th(IV) 14.5 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 Am(III) 24.5 0.000000002+00 0.00000000E+00 0.000000000000000 0.000000002+00 U(VT) 762 783 704 3.47561578E+00 1.02583551E-06 2.17706092E-01 9.18404325E-07 Np(V) 0.000000000+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 C104-(EL) 0.0000000E+00 0.0000000E+00 0.00000000±+00 0.0000000E+00 Phosphorus 1.50 0.000000000000+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Electron 74.6 -9.45337050E-16 -2.71700630E-15 -2.43246632E-15 0.0000000E+00 Charge 76.7 2575 Solution Parameters, Calculated 775 775 775 775 775 775 SOLUTION MASS 462.013014691340 grams 347.933330580303 H20 MASS grams TDS (g/kg) 327.877998698107 g/kgH20 Specified Solution Density $\hat{\gamma}_{i}$ 1188.81524828657 DENSITY kg/m^3 = g/l 775 Solution Parameters Based on Specified Density ?? 0.388633149984603 liters SOLUTION VOL 77) 77) 293.540795775029 a/1 743 Density based on TDS and NaCl solutions 1188 81524828657 a/1 Percent relative error vs NaCl density 0.000000000000000000000 % 722 783 SAC 1.00 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM 7 723 Species Name Molality Activity Act Coef Molarity Total Moles mg/liter Descriptor 738 285 H20 8.31870E-01 WATER 7.78092E-01 0.9354 1.93133E+01 4.96955E+01 8.952745+05 NaNp02C03(s) NaNp02C03 (s) 9.98931E+00 1.00000E+00 1.000 3.47562E+00 8.94318E+00 3.14841E+06 Na+ Na+ 5.61000E+00 5.289328+00 0.9428 1.95191E+00 5.02249E+00 1.15466E+05 7.4 C1c1-5.60673E+00 5.28679£+00 0.9429 1.95077E+00 5.01956E+00 1.77958£+05 CO3= CO3= 1.11398E-03 2.89293£-05 2.5969E-02 3.87591E-04 9.97318E-04 5.98482E+01 204 HC03-8003-1.02256E-03 3.78536£-04 0.3702 3.55784E-04 9.15475E-04 5.58596E+01 70: 794 OH-ÓН-2.40684E-05 1.30873E-05 0.5438 8.37419E-06 2.15478E-05 3 664708-01 -4.86E-D9 Np02 (C03) 2=-Np02 (C03)2=-7.13649E-07 1.84983E-11 2.5921E-05 2.48302E-07 6.38912E-07 2.48578E-01 9.95E-09 747 CO2 (ag) 2.18328E-07 6.33927E-07 CO2 (ag) 2.904 7.59637E-08 1.95464E-07 8.60232E-03 -3.58E-08 Np02C03-Np02C03-1.33654E-07 2.43125E-07 1.819 4.65026E-08 1.19657E-07 1.56E-12 3.93738E-02 794 Mp02 (C03) 3==-Np02 (C03) 3==-1.61312E-07 1.281932-16 7.9469E-10 5.61257E-08 1.44418E-07 6.48546E-02 1.971-08 - BOG NOO2+ 1.70494E-08 NpO2+ 3.389385-08 1.988 5.93207E-09 1.52639E-08 4.10671E-03 -9.14E-09 801 Н+ H+ 1.52979E-10 5.991295-10 3.916 5.32265E-11 1.36958E-10 1.38040E-07 -1.97E-08 SO2 NpO20H(ag)

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	Appendix N: Samp	ole Output File	"Np_NaCl_BN	I_LOG.OUT	•				
· · ·	••		-						
	NpO2 (OH) 2-	NpO2 (OH) 2-	3.61806E-13	1.08095E-13	0.2988	1.25884E-13	3.23915E-13	9.81663£-08	3.03E-08
~ (A	Na3H(CO3)2.2H20	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.96E+00
200	Na2CO3.H2O	_Thermonatrice	0.00000£+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.68E+00
200	Na2CO3.7H20Na2CO	3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.39E+00
507	Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000£+00	0.00000E+00	-3.36E+00
900 B	NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000£+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
e10	Na3NpO2(CO3)2(s)_DIS	SABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.32E+02
2.1.4			0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
2.2		Np020H(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.63E+00
5.1	NpO20H(aged)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.04E+00
 			0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.49E+02
213									
		2	9.8154						
21		= 9.2225							
0.00									
· · · ·	Equilibrium RH (%) =								
- 40	Ionic Strength (m) =								
2.4	Density, kg/m3 =			•					
d.42	Deubicy; xg/tb -								
	NOTES: - Water mol	lality: is mole f	Traction H2O in a	mieous phase					
· · · · · · · · · · · · · · · · · · ·									
		lity" and "activi	ity are gas part	ciai pressures					
	- *Descripto								
97 - 197		10 for species wi			e criterion)				
32		on Index for mine							
		ivity) for aque		very small co	centrations				
25		rtial pressure) f	or gases						
120									
	Total G/RT= -4.63	3619544E+03							
3 5.2									
	# inversions for bat		17						
تينا ج	18enchmark TITRATE Pr				molal NaCl F	MT V2.0			
641									
200	95.01.31 Am(III)-N	Na-C1-CO3-SO4-PO4		P91, RFFR92, RFF					
537	Pressure= 1.	.00000E+00 [=] A1	M Temperatu	re= 2.98E+0	2 [=] Kelvin				
(e*,)									
830	Elemental Abundances	s for Flash Probl	em						
~~~									
<i>.</i>		Ag. Molality	Aq. Molarity	Aq. mg/liter					
242									
340		1,11018446E+02	9.93922712E+01	1.00177470E+	05 Hydrogen				
÷		5.55178692E+01	4.97038762E+01	7.95232197E+				•	
2.5		5.61000623E+00	5.02251004E+00	1.15466351E+					
			0.00000000E+00	0.0000000E+0					
847			0.00000000E+00	0.0000000E+0					
843			0.0000000E+00	0.0000000E+0					
		5.60491242E+00	5.01794966E+00	1.77901369E+					
55 C		0.0000000E+00	0.0000000E+00	0.0000000E+					
211			2.72801516E-03	3.27661900E+0					
		00000000E+00							
< 74			0.0000000E+00	0.0000000E+					
2.5	0.00000000E+00	00+20000000000000	0.000000002+00	0.0000000E+	00 Neglon				
201 864	0.000000000000000000000000000000000000	0.000000000000000000000000000000000000	0.000000002+00 0.000000002+00	0.000000002+0 0.000000002+0	00 Neglon 00 Air				
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2013 264 365 964	0.000000000000000000000000000000000000	0.000000000000000000000000000000000000	0.000000002+00 0.000000002+00 0.000000002+00 0.000000002+00	0.000000000000000000000000000000000000	00 Neglon 00 Air 00 Boron 00 Bromine				Alexandra Transformer
203 204 504 504 504 504 504	0.000000000000000000000000000000000000	0.000000000000000000000000000000000000	0.000000002+00 0.000000002+00 0.000000002+00 0.000000002+00 0.0000000000	0.000000000000000000000000000000000000	00 Neglon 00 Air 00 Boron 00 Bromine 00 TracerEl				and a star since and
203 264 964 940 240 240	0.000000000000000000000000000000000000	0.000000000000000000000000000000000000	0.000000002+00 0.000000002+00 0.000000002+00 0.000000002+00	0.000000000000000000000000000000000000	00 Neglon 00 Air 00 Boron 00 Bromine 00 TracerEl				and the state of the
103 1854 1955 1955 1955 1955	0.000000000000000000000000000000000000	0.000000000000000000000000000000000000	0.000000002+00 0.000000002+00 0.000000002+00 0.000000002+00 0.0000000000	0.000000000000000000000000000000000000	00 Neglon 00 Air 00 Boron 00 Bromine 00 TracerEl 00 Th(IV)			Fe	and the state of the
203 264 964 940 240 240	0.00000000±00 0.00000000±00 0.00000000±00 0.0000000±00 0.00000000	0.000000000000000000000000000000000000	0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00	0.00000002+1 0.00000002+1 0.00000002+1 0.000000002+1 0.000000002+1 0.000000002+1 0.000000002+1 0.000000002+1	Neglon           Air           Boron           Bromine           TracerEl           Th(IV)           Am(III)           U(VI)				and the state of the
いい 1954 9959 1955 1955 1955	C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.0000000E+00 C.00000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.0000000E+00 C.00000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.000000000E+00 C.000000000E+00 C.00000000000E+00 C.000000000E+00 C.00000000000E+00 C.0000000000E+00 C.0000000000E+00 C.0000000000000000E+00 C.000000000000000E+00 C.000000000000000000 C.000000000000	0.000000000000000000000000000000000000	0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00	0.000000000000000000000000000000000000	Neglon           Air           Boron           Bromine           TracerEl           Th(IV)           Am(III)           U(VI)				AND THE PARTY OF AND
	C.00000000E+00 C 0.0000000E+00 C 0.0000000E+00 C 0.00000000E+00 C 0.00000000E+00 C 0.00000000E+00 C 0.00000000E+00 C 0.0000000E+00 C 0.0000000E+00 C	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00	0.00000002+1 0.00000002+1 0.00000002+1 0.000000002+1 0.000000002+1 0.000000002+1 0.000000002+1 0.000000002+1	Neglon           Air           Boron           Bromine           TracerEl           Th(IV)           Am(III)           U(VI)           Np(V)				
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いい (1974年1975年1975年1975年1975年1975年1975年1975年1975	C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.000000000E+00 C.000000000E+00 C.00000000E+00 C.000000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.000000000E+00 C.00000000E+00 C.000000000E+00 C.00000000000000E+00 C.0000000000000000000000000000000000	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 1.740614272-06 0.00000002+00 0.00000002+00 0.00000002+00	0.00000002+4 0.00000002+4 0.00000002+4 0.000000002+4 0.000000002+1 0.000000002+1 0.00000002+4 4.126094802-0 0.00000002+1 0.00000002+1	Negion           Air           D0         Boron           D0         Boron           D0         Bromine           D0         TracerEl           D0         An(II)           D0         U(VI)           D1         Mp(V)           D0         Cl04-(EL)           D0         Phosphorus           D0         Electron	5			and the state of t
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2012 7844 9555 9567 7057 7057 8000 8000 8000 8000 8000 800	0.00000000000000000000000000000000000	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 1.74061427E-06 0.00000002+00 0.00000002+00 0.00000002+00 2.74631980E-15 6 grams 12 g/kgH20 59 kg/m^3 = 1.fied Density 23 liters 19 g/l 1188.83	0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	<pre>33 NegIon 30 Air 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 Am(III) 30 U(VI) 31 Mp(V) 30 Cl04-(EL) 30 Phosphorus 30 Electron 30 Charge 371</pre>	5			
2008 2008 2009 2009 2009 2009 2009 2009	0.00000000000000000000000000000000000	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 1.74061427E-06 0.00000002+00 0.00000002+00 0.00000002+00 2.74631980E-15 6 grams 12 g/kgH20 59 kg/m^3 = 1.fied Density 23 liters 19 g/l 1188.83	0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	<pre>33 NegIon 30 Air 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 Am(III) 30 U(VI) 31 Mp(V) 30 Cl04-(EL) 30 Phosphorus 30 Electron 30 Charge 371</pre>				
2012 1954 1955 1957 1957 1957 1957 1957 1957 1957	0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.000000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.000000000E+00 0.000000000000000000 0.00000000000	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 1.74061427E-06 0.00000002+00 0.00000002+00 0.00000002+00 2.74631980E-15 6 grams 12 g/kgH20 59 kg/m^3 = 1.fied Density 23 liters 19 g/l 1188.83	0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	<pre>33 NegIon 30 Air 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 Am(III) 30 U(VI) 31 Mp(V) 30 Cl04-(EL) 30 Phosphorus 30 Electron 30 Charge 371</pre>				
200 7544 564 765 765 765 765 765 765 77 77 75 75 75 77 77 77 77 77 77 77 77	0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.000000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.000000000E+00 0.000000000000000000 0.00000000000	0.000000000000000000000000000000000000	0.00000002=00 0.0000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.0000000000	0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	<pre>33 NegIon 30 Air 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 Am(III) 30 U(VI) 31 Mp(V) 30 Cl04-(EL) 30 Phosphorus 30 Electron 30 Charge 371</pre>	5			
2007 7544 9455 8555 8651 8652 8652 8652 8652 8652 8777 8752 8752 8752 8752 8752 8752 87	0.00000000000000000000000000000000000	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 1.74061427E-06 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 2.74631980E-15 59 grams 12 g/kgH20 59 kg/m ³ = 1 fied Density 23 liters 19 g/l 1 ations 1188.8; 15 sity 0.000000	0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	<pre>33 NegIon 30 NegIon 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 U(VI) 30 Am(III) 30 U(VI) 30 Cl04-(EL) 30 Phosphorus 30 Electron 30 Charge 3/1 0 %</pre>				
201 7544 955 955 955 955 955 955 955 955 955	C.00000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.00000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.0000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.00000000E+00 C.0000000000 C.00000000000 C.00000000	0.000000000000000000000000000000000000	0.00000002=00 0.0000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.00000002=00 0.0000000000	0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	<pre>33 NegIon 30 Air 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 Am(III) 30 U(VI) 31 Mp(V) 30 Cl04-(EL) 30 Phosphorus 30 Electron 30 Charge 371</pre>	Total Moles	Molarity	mg/liter	
(1) 7544 965 755 755 755 755 755 755 755 755 755 7	0.00000000000000000000000000000000000	0.00000000E+00 0.000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000000	0.00000002+00 0.0000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 1.74061427E-06 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 2.74631980E-15 1.6 grams 12 g/kgH20 59 kg/m^3 = 1.5 grams 12 g/kgH20 59 kg/m^3 = 1.5 liters 1.8 l	0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	<pre>33 NegIon 30 Air 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 U(VI) 30 Cl04-(EL) 30 Electron 30 Electron 30 Charge 30 St 30 St 3</pre>	Total Moles			
2012 7524 9455 7555 7555 7555 7555 7555 7555 755	0.00000000000000000000000000000000000	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 2.74631980E-15 6 grams 12 g/kgH20 59 kg/m ³ = 1 fied Density 23 liters 19 g/l 1 stions 1188.8: 1 sity 0.000000 (STEM Molality 8.318812-01	0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.00000002+ 0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	03 NegIon 10 Air 10 Boron 10 Bromine 10 Bromine 10 TracerEl 10 Th(IV) 10 Am(III) 10 U(VI) 10 Mp(V) 10 Cl04-(EL) 10 Phosphorus 10 Electron 10 Charge 10 S Act Coef 0.9354	Total Moles 1.93221E+01	4.96957E+01	8 95277E+05	
(1) 7584 965 755 765 765 765 765 777 775 775 775 7	0.0000000E+00       0         0.000000E+00       0         0.00000E+00       0         0.00000E+00       0         0.00000E+00       0         0.00000E+00       0         0.00000E+00       0	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.000000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.000000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.000000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.0000000000000000000 0.0000000000	0.000000000000000000000000000000000000	<pre>33 NegIon 30 Air 30 Boron 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 U(VI) 30 Cl04-(EL) 30 Cl04-(EL) 30</pre>	Total Moles 1.93221E+01 3.47562E+00	4.96957E+01 8.93914E+00	8 95277E+05 3 14699E+06	
(1) (2) (2) (2) (2) (2) (2) (2) (2) (2) (2	0.0000000E+00       0         0.000000E+00       0         0.0000000E+00       0         1.06779239E-15       -3         Solution Parameter       SOLUTION WASS         TDS       Density based on T         Percent relative e       TABLE OF CONCENTRATI         Species Name       H20         NaNp02C03(s)	0.00000000E+00 0.000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.0000000E+01 0.000000E+01 0.000000E+01 0.000000E+01 0.000000E+01 0.000000E+01 0.000000E+01 0.000000E+01 0.000000E+01 0.0000000E+01 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.0000000E+00 0.000000000E+00 0.0000000000	0.00000002+00 0.0000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 1.74061427E-06 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 2.74631980E-15 2.74631980E-15 3.9 grams 2 g/kgH20 59 kg/m^3 = 1 fied Density 23 liters 9 g/l 1 tions 1188.8: 1 sity 0.00000 (STEM Molality 8.31881E-01 9.98478E+00 5.61001E+00	0.00000002+ 0.00000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.000000002+ 0.0000000000	<pre>33 NegIon 30 NegIon 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 U(VI) 30 Cl04-(EL) 30 Electron 30 Electron 30 Charge 31 00 % 32 0 % 33 0 % 34 0 0 % 35 0 0 % 35 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0</pre>	Total Moles 1.93221E+01 3.47562E+00 1.95279E+00	4.96957E+01 8.93914E+00 5.02251E+00	8 95277E+05 3 14699E+06 1 15466E+05	
(1) 7544 9445 7555 7557 7557 7557 7557 7557	0.0000000E+00       0         0.000000E+00       0         0.00000E+00       0         0.00000E+00       0         0.00000E+00       0         0.00000E+00       0         0.00000E+00       0	0.000000000000000000000000000000000000	0.00000002+00 0.0000002+00 0.0000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.000000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.000000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.000000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.00000002+00 0.0000000000000000000 0.0000000000	0.000000000000000000000000000000000000	<pre>33 NegIon 30 Air 30 Boron 30 Boron 30 Bromine 30 TracerEl 30 Th(IV) 30 Am(III) 30 U(VI) 30 Cl04-(EL) 30 Cl04-(EL) 30</pre>	Total Moles 1.93221E+01 3.47562E+00	4.96957E+01 8.93914E+00	8 95277E+05 3 14699E+06	

64.0

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT" нсоз-1.04073E-03 3.85192E-04 0.3701 HCO3-3.62268E-04 9.31738E-04 5.68519E+01 242 ÓН-4.24988E-05 2.31125E-05 OH-0.5438 1.47935E-05 3.80482E-05 6.47098E-01 -6.18E-08 No02 (C03) 2=-23.16 Np02 (C03) 2=-1.28137E-06 3 374478-11 2.59455-05 4.46032E-07 1.14718E-06 4.46327E-01 4 81E-08 4.13999E-16 Np02 (C03) 3==-5.19502E-07 4.65098E-07 200 Np02 (C03) 3==-7.9692E-10 1.80834E~07 2.088648-01 1.06E-07 3.65269E-07 80-CO2 (ag) C02 (ag) 1.25799E-07 2.904 4.37894E-08 1.12625E-07 4.95659E-03 -3.39E-07 1/0.0 Np02C03-ND02C03-1 336888-07 2.43151E-07 1 819 4.65356E-08 1.196882-07 3.93840E-02 1.10E-12 e de 9.49498E-09 1.88634E-08 ND02+ No02+ 1.987 3 30512E-09 8.50064E-09 2.28707E-03 -4.03E-08 8442 H+ 8.66954E-11 3.39269E-10 3.913 3.01779E-11 H+ 7.76164E-11 7.82296E-08 -1.47E-07 Np020H(ag) 30 NpO20H (ag) 1.68316E-10 1.68316E-10 1.000 5.85892E-11 1.50689E-10 4.31052E-05 1 048-07 1.876272-13 ND02 (0H) 2-NoO2 (OII) 2-6.28105E-13 0.2987 2 18638E+13 5.62328E-13 1.70420E-07 2.44E-07 202 Na3H(C03)2.2H20_ 0.00000E+00 1.00000E+00 1.000 Trona 0.00000E+00 0.00000F+00 0.00000E+00 -4.70E+00 Thermonatrite 0.00000E+00 1.00000E+00 0.00000E+00 Na2C03, H20 1.000 0.00000E+00 0.000005+00 +3 435+00 4.6 Na2CO3-Heptahydrate 1.00000E+00 Na2CO3.7H20 0 000005+00 1 000 0 00000E+00 0.00000E+00 0.00000E+00 -3.14E+00 0.00000E+00 1.00000E+00 995 Na2CO3.10H20 Natron 1.000 0.00000E+00 0.000002+00 0.00000E+00 -3.10E+00 Nahcolite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 3.): NaHCO3_____ 0.00000E+00 -2.29E+00 303 1.00000E+00 NaC1 Halite 0.00000E+00 1,000 0 00000E+00 0.00000E+00 0.00000E+00 -1.24E-01 Na3Np02 (CO3) 2 (s)_DISABLED_DISABLED 0.00000E+00 1.00000E+00 1.000 226 0.00000E+00 0.000005+00 0.00000E+00 -9.31E+02 NaOH(ag).....to.titrate.base.only 0.00000E+00 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 -2 945+02 1.00000E+00 NpO2OH(amor)_____NpO2OH(amor) 0.000008+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.64E+00 1.00000E+00 Np020H (aged) 0.00000E+00 NpO2OH (aged) 1.000 0.00000E+00 0.00000E+00 0.00000£+00 -3.05E+00 HCl(aq)...., to.titrate.acid.only 0.00000E+00 0.00000E+00 1.000 1.2 0.00000E+00 0.00000E+00 0.00000E+00 -2 49E±02 pmH = -log[m(H+)]10.0520 6.10 pH = -log[a(Hr)]9.4695 . 7 1.241325 Osmotic Coefficient= 12 77.812731 Equilibrium RH (%) = ). Sty Ionic Strength (m) = 5.612017 321. 1188.81 Density, kg/m3 NOTES: - Water 'molality' is mole fraction H2O in aqueous phase - Gas 'molality' and 'activity' are gas partial pressures 923 -"Descriptor" means: -dG/RT/1n10 for species with nonzero concs. (convergence criterion) *Saturation Index for minerals, SI=log10(IAP/Ksp) *logl0(activity) for aqueous species with very small concentrations 120 *log10(partial pressure) for gases 4. j. j. Total G/RT= -4.63721298E+03 Flashing Titration # # inversions for batch pblm 2.11 8 322 23 222 Benchmark TITRATE Problem, LOG10 option; Np(V)02 with CO3 in 5.61molal NaCl - FMT V2.0 612 DATABASE: HMW84/FW86; Np(V)-Na-C03-OH-C1-C104 (NR94): 95.01.31 Am(III)-Na-C1-C03-S04-P04 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94) 1.5 1.00000E+00 [=] ATM 335 **Pressure**= Temperature= 2.98E+02 [=] Kelvin 331 323 Elemental Abundances for Flash Problem 22.5 64.5 Total Moles Ag. Molality Ag. Molarity Ag. mg/liter a.; ; 4.11 3.86695692E+01 1.11018496E+02 1.00177932E+05 Hydrogen 9.93927291±+01 343 4.97075822E+01 3.67172215E+01 5.55217779E+01 7.95291491E+05 Oxygen 244 5.42967348E+00 5.02253469E+00 5.61001045E+00 1.15466917E+05 Sodium 500 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Potassium 5.C.? 0.0000000E+00 0.00000002+00 0 00000005+00 0.000000000+00 Magnesium <u>ج</u>يت 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Calcium 3.15 1.95138405E+00 5 60233091E+00 5.01565935E+00 1.77820171E+05 Chlorine 444 0.00000005+00 0.00000002+00 0.00000005+00 Sulfur 3.47712639E+00 4.34048558E-03 3.88595344E-03 201 4.66741868E+01 Carbon 251 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Posion 55 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Necion  $\zeta \leq \zeta$ 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 Air 44.4 0.00000005+00 0.0000000E+00 0.0000000E+00 Boron 30. 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Bromine 22.0 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 TracerEl 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 Th(IV) 44.4 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Am(TTT) 64.2 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 U(VI)  $\langle \sigma \rangle$ 3.47561578E+00 3.60501967E-06 3.22750493E-06 7.65074233E-01 Np(V)383 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 C104-(27.) 302 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 Phosphorus 962 0.0000000000+00 0.0000000E+00 0.00000000E+00 Electron G. -4.02027671E-16 -1.15420235E-15 -1.03333521E-15 0.0000000E+00 Charge 1.0 series Solution Parameters. Calculated 357 SOLUTION MASS 462.514079623513 grams 902 Xor H20 MASS 348.316456438668 grams TDS(q/ka)327.855951316366 g/kgH20 Specified Solution Density 37 1188.80395005085 DENSITY  $k\alpha/m^3 = \alpha/l$ 27% 377 Solution Parameters Based on Specified Density 978 478 477 0.389058330100373 SOLUTION VOL liters 293.523141261063 TOS q/1 975 379 Density based on TDS and NaCl solutions 1188.80395005085  $\sigma/1$ Percent relative error vs NaCl density 0.00000000000000000000 % 32. 321

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

CONTRACTOR FOR BATCH SYSTEM

Dispetition         Provintion         Participation         Participation         Participation         Participation           Dispetition         A. 2000101		TABLE OF CONCENTRA	TIONS FOR BATCH S	YSTEM						
<pre>11 H00</pre>		Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
<pre>c cl-</pre>	23									
C 03* 03* 03* 03* 03* 03* 03* 03* 03* 03*									1.15467£+05	
Display         NO3-         NO3- <thno3-< th="">         NO3-         NO3-         &lt;</thno3-<>										
<pre>17 dr. 0 + + + + + + + + + + + + + + + + + +</pre>										
<pre>     Pact(2013):- Pact(201</pre>										
<pre>     Ap22(C03):s B222(C03):s 1.37732-60 1.1020E-15 0.001E-10 4.07754-67 1.32306-60 3.127751-60 4.100-00     C0324, 00000000 1.00000000 3.10312-00 4.0754-67 1.32306-60 3.127751-60 4.100-00     Pa200 Model 1.1020E-00 1.0000000 3.10200-00 1.10200-00 3.12020-00 3.12020-00 3.12020-00     Pa200 Model 1.1020E-00 1.00000000 1.00000000 1.00000000 1.00000000</pre>										
<pre>cr d21eq: C021eq: C021eq:</pre>										
<pre>mp. pp. 2000 - NB00001 - 1.337378-77 2.41878-77 1.818 4.45677-08 1.19326-1 2.32642 - 2.32642 pp. pp. 2000 - 2.42642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 pp. pp. 2000 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 pp. 2000 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2.34642 - 2</pre>										
Dysc/r         Number         Support         Support <thsupport< th=""> <thsupport< th=""> <thsup< th=""><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th></thsup<></thsupport<></thsupport<>										
<pre>min text</pre>										
<pre>31</pre>			-		2.12840E-10	3.909	1.89655E-11			
<pre>1</pre>	1000				1.64493E-10	1.000	5.72955E-11			
<pre>1: Macco Maco</pre>	101			9.78743E-13	2.92306E-13	0.2987	3.409122-13	8.76250E-13		
<pre>11 Marcol 7020</pre>	1022			0.00000E+00	1.00000E+00		0.00000E+00	0.0000E+00	0.00000E+00	-4.48E+00
<pre>1: haccol.0020Matter 0 0.000000-00 1.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.000000-00 0.000000-00 0.000000-00 0.0000000-00 0.000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.0000000-00 0.000000</pre>									0.00000E+00	-3.22E+00
Mach20										
<pre>11 Hath_CCC12[i]_UDABLED_DIAMARED_0_0000000000000000000000000000000000</pre>										
<pre>     AbaCV 2013 / 12 JUSANLED DISANLED 0.000000-00 1.0000 0.00000-00 1.000 0.000000-00 0.000000-003.245-00     AbaCV 2014 JUSANLED DISANLED 0.000000-00 1.00000-00 1.000 0.000000-00 0.000000-00 0.000000-00     AbaCV 2014 JUSANLED VERSION OF THE ABACV 201</pre>		Narcos								
<pre>50 NacWing]to.titrate.hase.only 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.00000002+0 0.00000002+0 0.0000002+0 0.0000002+0 0.0000002+0 0.000</pre>										
<pre>11 mpC201(macr)</pre>										
<pre>C: bpC200(spec)</pre>	1.11	NpO2OH (amort)	NoO2OH(amor)							
<pre>31 Mrtisg)to.titrate.acid.only 0.0000000-00 0.000000-00 0.000000-00 0.000000-00 0.000000-00 -2.092-02 31 Mrtisg)to.titrate.acid.only 0.0000000-00 0.0000000-00 0.0000000-00 -2.092-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02 32.992-02</pre>	<u></u>	NpO20H (aged)	Np020H(aged)							
<pre>11 ppt = -log[m[H-1]</pre>	1212	HCl(ag)to.t:	trate.acid.only							
<pre>i pr -logia/t-1] = 9.6713 Osmonic Coefficients : 1.43149 Osmonic Coefficients : 1.43149 Tomic Exerciption = 1.43149 Tomic Exerciption = 1.43149 Presity, Myral = 1188.00 NTTE: - Mater "molality' and "scivity" are gas partial pressures - Coefficients : 1.1000 - Tobil Scivity' for Agence Coefficient : 1.1001 - Tobil Scivity' for Agence : 1.1001 - Tobil Moles Ag. Molality Ag. Molarity Ag. mg/liter - Scill'' Tobil Moles : 1.1001 - Scill'' Tobil Scivity' for Agence : 0.000000000-00 - 0.00000000-00 - 0.00000000-00</pre>	191A -							-		
<pre>1. Domotic Coefficient 1.24119 Spullburght B1 (1) = 7.24733 Tonic Strength Int = 5.431297 Demaity, AgrAl = 1188.60 Unic Strength Int = 5.431297 Demaity, AgrAl = 5.431297 Demaity, AgrAl</pre>			:	≈ 10.26 <b>4</b> 0						
<pre>Styliferium SM (W) = 77.81733 Tonic Strength (m) = 5.63227 Pensity, MgrAl = 1188.00 NUTES:</pre>										
<pre>Note: strength (m) = 5.61227 Density, Myn1 = 1188.80 NOTE: - Water 'molality' is mole fraction H2O in squeous phase</pre>										
<pre>11 Demaity, MyrAl = 1188.0 WTE: - Water "molality" is mole fraction H2O in squeous phase</pre>										
<pre>NOTES: - Water "molality" is mole fraction H20 in equeous phase</pre>	area Area	Density bara?								
MOTEs:         • Water "molality" is mole fraction R20 in squeeus phase           • Gest "molality" and "saturity" and "saturity		Density, Ky/10	1100.00							
<pre>- cgs 'solidity' and 'sctivity' are gas partial pressures - 'dS/RY/hD1 for species with monzero cons. (convergence criterion) - 'dsituration index for mainteria. St-iog(12R/KSp) - 'hog10(sctivity) for squeens species with very small concentrations - 'hog10(sctivity) for squeens species with concentrations - 'hog10(sctivity) for squeens - 'hog10(sctivity) for squeens squeens squeens squeens for squeens squeens squeens for squeens - 'hog10(sctivity) for squeens - 'hog10</pre>		NOTES: - Water "mo	lality" is mole	fraction H2O in	aqueous phase					
- 'Descriptor' means: "diff'/linb for species with nonzero concs. (convergence criterion) "saturation Index for minerals. Srilog10(127/Kpp) "hop10(stitly) for aqueous species with very small concentrations "hop10(stitly) for aqueous species with concentrations "hop10(stitly) for aqueous species with concentrations hop10(stitly) for aqueous species withop10(stitly) for aqueous species withop10(	1.2									
<pre>*d5/RT/In10 for species with nonzero concs. (convergence criterion) *dsturation index for interrals, SF1001(12P/Rep) *log10[activity] for aqueous species with very small concentrations *log10[activity] for aqueous species with very species species species species with very species with very species speci</pre>	12				•					
<pre>     'logl0(activity) for aqueous species with very small concentrations     'logl0(partial pressure) for gases     'logl0(partial</pre>		•dG/RT/lr	10 for species w	ith nonzero conc	s. (convergence	criterion)				
<pre>     *10g101partial pressure) for games     *10g101partial pressure) for games     Total G/RT    -4.638602840-03     Flashing Tirration f</pre>	026	*Saturati	on Index for min	erals, SI≂log10(	LAP/Ksp)					
Total G/RT-       -4.63866284E-03         Pisahing Titration f       9         f investions for betch pblm       23         Total MARKE Froblem, LOGIO option; Ng(V)C2 with CO3 in 5.61mclal NaCl Pff V2.0         DATABAS: BM64/FM65; Ng(V)-Na-Cl-CO3-OH-Cl-CLG4 (MR94);         Sol.31 Am(III)-Na-Cl-CO3-SO4-PC4 (FERRES), RFF90, RFF92, RFF94, RFF94)         Pressurer       1.00000E-00 [.] AM         Total Moles       Aq. Molality       Aq. molarity         Ag. Molality       Aq. Molarity       Aq. mg/liter         Total Moles       Aq. Molality       Aq. mg/liter         1 ST052148FeO1       1.1018564E-02       9.3931703E-03       1.00178578E-05       Mydrogen         1 ST052148FeO1       0.10000000E-00       0.000000E-00       0.000000E-00       0.000000E-00       0.000000E-00         0 0.000000E-00       0.000000E-00       0.000000E-00       0.000000E-00       0.00000E-00       0.00000E-00         0 0.000000E-00       0.000000E-00       0.000000E-00       0.00000E-00       0.00000E-00       0.00000E-00         0 0.00000E-00       0.00000E-00       0.00000E-00       0.00000E-00       0.00000E-00       0.0000E-00         2 0.00000E-00       0.00000E-00       0.00000E-00       0.0000E-00       0.0000E-00       0.0000E-00         2 0.000					.very small con	centrations				
<pre>C20 Total G/RT= -4.63866248-03 Flashing Tiration f 9 Flashing</pre>		*logi0(pa	irtial pressure)	for gases						
021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       9         021       1.10185642-02       9.33317052-01         021       1.67357082-01       5.52714112-01       4.71228178-01         0.37570822-01       5.5271412-01       4.71228178-01       7.35736328-05         0.37570822-01       5.5271412-01       4.71228178-01       7.35736328-05         0.37570822-01       5.5271412-01       4.71228178-01       7.35736328-05         0.37570822-01       5.0234642-03       5.32146542-03       7.35376328-05         0.37570822-01       5.0000000-00       0.00000000-00       0.00000000-00         0.000000000-00       0.000000000-00       0.000000000-00       0.000000000-00         0.000000000-00       0.000000000-00       0.000000000-00       0.000000000-00<										
<pre>23 inversions for batch pblm 23 iBenchmark TTRME Problem, LG10 option; Ny(V102 with C03 in 5.61molal NaCl PHT V2.0 iBenchmark TTRME Problem, LG100-G01+C1-c104 (M894); 95.01.11 Am(III)-Na-C1-C03-G04-C1-c104 (M894); 95.01.11 Am(III)-Na-C1-C03-G04-C1-c104 (M894); 15 iEmental Abundances for Flash Problem iEmental Abundances for Flas</pre>										
32         Descharter TITMATE Problem. LOGIO option: hp(v)C2 with CC3 in 5.6lmolal Nac1 PMT V2.0           30 DATABASE: mp604/rM66: hp(v)-An-C0-C0-C0-Lot (N894):           32         Pressurer 1.00000E+00 [= ATM Temperaturer 2.98E+02 [=] Kelvin           32         Elemental Apundances for Flash Problem           33         Art Molarity Aq. Molarity Aq. mp/liter           34         3.6735708F+01 5.55273411E+01 4.97128372F+01 7.953782F05 Mydrogen           3.6735708F+01 5.55273411E+01 4.97128372F+01 7.95378328+05 Sodium           3.6.00000005F+00 0.00000000E+00 5.000000E+00 0.0000000E+00 0.000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.0000000E+00 0.000000E+00 0.0000000E+00 0.000000E+00 0.00000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.00000E+00 0.000000E+00 0.00000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.00000E+00 0.000000E+00				23						
33       DXTRASE: B098/FM86: B0(V)-FAc-C03-OFC-L-C104 (M894):         95.01.31 Am(III)-MacC1-C03-S04-P04 (FRSRSP, RF96).P31, MFF92, RFF94, REF94)         Pressure: 1.00000E+00 [=] ATM Temperature: 2.98E+02 [=] Kelvin         21       Total Moles Aq. Molality Aq. Molarity Aq. mg/liter         31       DXT214EE-01 1.1101854E+02 9.93933709E+01 1.00178579E+05 Hydrogen         3.6705214EE-01 3.577341LE-04 97128571E+01 7.57378512E+05 Sodymen         3.6705214EF-01 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00					th CO3 in 5.61m	olal NaCl T				
25       95.01.31       Ap(111)-Na-01-003-SO4-PO4 (FRSR89, FRF90, F91, FRFF94, RFF94)         Pressurer       1.00000F+00 [= ) ATM       Temperature*       2.98E+02 [=] Kelvin         10000F       Total Moles       Aq. Molality       Aq. Molarity       Aq. mg/liter         10000F       0.11008664F*02       9.33331705E+01       1.00178579E+05       Hydrogen         100000F       0.0000000F*00       0.0000000F*00       0.0000000F*05       Sodium         1000000F       0.0000000F*00       0.0000000F*00       0.0000000F*00       Sodium         1000000F       0.0000000F*00       0.0000000F*00       0.0000000F*00       Sodium         1000000F       0.0000000F*00       0.0000000F*00       Sodium       Sodium         11       Sidius       Sidius       Sidius       Sidius       Sidius         11       Sidius       Sidius       Sidius       Sidius       Sidius         11       Sidius       Sidius       Sidius       Sidius       Sidius       Sidius         11       Sidius       Sidius       Sidius       Sidius       Sidius       Sidius         11       Sidius       Sidius       Sidius       Sidius       Sidius       Sidius         11       Sidius </th <th></th>										
1/1         Elemental Abundances for Flash Problem           1/2         Total Moles         Aq. Molality         Aq. mg/liter           1/2         3.870521485+01         1.10185645+02         9.93937095+01         1.001785795+05         Mydrogen           1/2         3.673697085+01         S.552734112+01         4.971285778+02         Mydrogen           1/2         3.673697085+01         S.552734112+01         4.971285778+02         S.00000002+00           0.0000000000000         0.0000000000000000         0.00000000000000000000000000000000000		95.01.31 Am(III)-	Na-C1-CO3-SO4-PO	4 (FRSR89, FRF90,	P91, RFFR92, RFF9	4.RRFF94)				`````
Elemental Abundances for Flash Problem           Total Moles         Aq. Molality         Aq. Molarity         Aq. mg/liter           36         J.673697085-01         J.510118564E+02         9.93931709E+01         1.00179579E+05         Hydrogen           37         J.673697085-01         S.55271411E+01         4.971245378-01         7.95375812E+05         Sodguen           37         S.4314755-00         S.000000000000000000000000000000000000	035	Pressure= 1	00000E+00 [=] A	TM Temperatu	re= 2.98E+0	2 [=] Kelvin				
Total Moles         Aq. Molality         Aq. Molarity         Aq. mg/liter           3.473521462+01         1.11018564E+02         9.93933709E+01         1.00178579E+05         Mydrogen           3.47359708E+01         5.5527341E+01         4.97128517E+01         7.95378812E+05         Sodyman           0.0000000E+00         0.0000000E+00         0.0000000E+00         0.000000E+00         0.000000E+00           0.0000000E+00         0.0000000E+00         0.000000E+00         0.000000E+00         Calcum           0.000000E+00         0.000000E+00         0.000000E+00         Calcum         Calcum           0.000000E+00         0.000000E+00         0.000000E+00         Calcum           0.000000E+00         0.000000E+00         0.00000E+00         Calcum           0.000000E+00         0.000000E+00         0.000000E+00         Sulfur           0.000000E+00         0.000000E+00         0.000000E+00         Pastan           0.000000E+00         0.000000E+00         0.000000E+00         Pastan           0.000000E+00         0.000000E+00         0.000000E+00         Pastan           0.000000E+00         0.000000E+00         0.000000E+00         Pastan           0.000000E+00         0.000000E+00         0.0000000E+00         Pastan		a								
No.       Total Moles       Aq. Molality       Aq. Mg/liter         No.       Total Moles       Aq. Mg/liter         No.       Status       No.       No.         No.       Status       Status       No.       No.         No.       Status       Status       No.       No.       No.         No.       Status       Status       No.       No.       No.         No.       Status       Status       No.       No.       No.       No.       No.         No.       Status       Status       No.       No.       No.       No.       No.       No.       No.         No.       Status       No.       No. <t< th=""><th>138</th><th>Elemental Abundance</th><th>S IOF FIASH FROD.</th><th>1 em</th><th></th><th></th><th></th><th></th><th></th><th>· • •</th></t<>	138	Elemental Abundance	S IOF FIASH FROD.	1 em						· • •
144       3.87052148E+01       1.1018564E+02       9.83831709E+01       1.00178579E+05       Hydrogen         123       3.67369709E+01       5.55273411E+01       4.97128537E+01       7.95375832E+05       Sodum         123       5.43147473E+00       5.6101696E+00       5.0225690E+00       1.13467727E+05       Sodum         124       0.0000000E+00       0.000000E+00       0.000000E+00       0.000000E+00       Calconoversion         124       0.000000E+00       0.000000E+00       0.000000E+00       Calconoversion       Calconoversion         125       0.000000E+00       0.000000E+00       0.000000E+00       Calconoversion       Calconoversion         124       0.000000E+00       0.000000E+00       0.000000E+00       Calconoversion       Sudu         124       0.000000E+00       0.000000E+00       0.000000E+00       Calconoversion       Sudu         125       0.0000000E+00       0.000000E+00       0.000000E+00       Calconoversion       Sudu       Sudu         125       0.000000E+00       0.000000E+00       0.000000E+00       Sudu       Sudu       Sudu         126       0.000000E+00       0.000000E+00       0.000000E+00       Sudu       Sudu       Sudu       Sudu       Sudu	1.55	Total Moles	Aq. Molality	Ag. Molarity	Ag mg/liter					`
3.67369700E>01       5.5273411E>01       4.9712837E>01       7.93375832E>05       Sodium         3.67369700E>01       5.40147475P>00       5.61001696E>00       1.15467727E>05       Sodium         3.6736970E>01       0.0000000E>00       0.0000000E>00       0.0000000E>00       0.0000000E>00       0.0000000E>00         4.70       0.0000000E>00       0.0000000E>00       0.0000000E>00       0.000000E>00       0.000000E>00         4.71       0.000000E>00       0.000000E>00       0.000000E>00       0.000000E>00       0.000000E>00         6.0000000E>00       0.000000E>00       0.000000E>00       0.000000E>00       0.000000E>00       0.000000E>00         0.000000E>00       0.000000E>00       0.000000E>00       0.000000E>00       0.000000E>00       0.000000E>00         0.0000000E>00	:40		-	-	-					
3:3       5.41147475F-00       5.61001696E-00       5.02256990E-00       1.15467727E-05       Solium         3:4       0.0000000E-00       0.0000000E+00       0.0000000E+05       Solium         4:4       0.000000E+00       0.0000000E+00       0.0000000E+00       Colourse         4:4       0.000000E+00       0.000000E+00       0.000000E+00       Calcium         4:4       0.000000E+00       0.000000E+00       0.000000E+00       Sulfur         4:3       1.4774655E+00       6.417139E8+01       Catbon         7:9       0.000000E+00       0.000000E+00       0.000000E+00       Air         7:0       0.000000E+00       0.000000E+00       0.000000E+00       Air         7:1       0.000000E+00       0.000000E+00       0.000000E+00       Air         7:2       0.000000E+00       0.000000E+00       0.000000E+00       Air         7:1       0.000000E+00       0.000000E+00       0.0000000E+00       Air		3.87052148E+01	1.11018564E+02	9.93933709E+01	1.00178579E+0	5 Hydrogen				
243       0.00000005F-00       Calcium         244       1.55190099F+00       5.59865759F+00       5.0124002F+00       0.00000005F-00       Calcium         245       0.0000000F+00       0.0000000F+00       0.0000000F+00       Calcium         243       3.47776555F+00       6.18147537F-03       5.53418664F-03       6.6471139E+01       Calcium         253       0.0000000F+00       0.0000000F+00       0.0000000F+00       0.0000000F+00       0.0000000F+00       0.0000000F+00         254       0.0000000F+00       0.0000000F+00       0.0000000F+00       0.0000000F+00       Acoon0000F+00       Acoon0000F+00         255       0.0000000F+00       0.0000000F+00       0.0000000F+00       Boron       Boron         255       0.0000000F+00       0.0000000F+00       0.0000000F+00       Boron       Acoon0000F+00       Acoon0000F+00       Acoon000F+00       Acoo	943									
140       0.00000005400       0.00000005400       0.0000005400       Magnesium         140       0.0000005400       0.0000005400       0.0000005400       0.0000005400       0.0000005400         1.951900992400       5.598657592400       5.012400022400       1.777046182405       Chlorine         142       0.0000005400       0.00000002400       0.00000002400       0.00000002400       0.00000002400         143       0.477768555400       0.00000002400       0.00000002400       0.00000002400       0.00000002400         150       0.0000002400       0.00000002400       0.00000002400       0.00000002400       0.0000002400         151       0.0000002400       0.00000002400       0.00000002400       0.0000002400       Neglon         152       0.00000002400       0.00000002400       0.00000002400       Neglon       Air         152       0.00000002400       0.00000002400       0.0000002400       Neglon       Air         154       0.0000002400       0.00000002400       0.00000002400       Neglon       Air         155       0.00000002400       0.00000002400       0.00000002400       Neglon       Air         155       0.00000002400       0.00000002400       0.00000002400       Neglon       Air     <	233									
644       0.000000005+00       0.00000005+00       0.0000005+00       Calcium         647       1.951900997+00       5.998657595+00       5.012400022+00       1.777046185+05       Chlorine         643       3.477768555+00       6.181473378-03       5.534188462-03       6.647113982+01       Carbon         753       0.00000005+00       0.000000005+00       0.000000005+00       0.00000000000000       PosIon         753       0.00000005+00       0.000000005+00       0.000000005+00       0.000000000000000       NegIon         754       0.00000005+00       0.00000005+00       0.00000005+00       0.00000005+00       NegIon         754       0.00000005+00       0.00000005+00       0.00000005+00       0.00000005+00       NegIon         755       0.00000005+00       0.00000005+00       0.00000005+00       No0000005+00       No0000005+00         755       0.00000005+00       0.00000005+00       0.00000005+00       No0000005+00       TraceEl         756       0.00000005+00       0.000000005+00       0.000000005+00       No0000005+00       No0000005+00         757       0.00000005+00       0.000000005+00       0.000000005+00       No0000005+00       No0000005+00         757       1130571155-15       -3.243689285-15 <td></td>										
343       1.951900992+00       5.59865759E+00       5.01240002E+00       1.77704618E+05       Chlorine         343       0.0000000E+00       0.0000000E+00       0.0000000E+00       S.3341854E-03       6.471139EE+01       Carbon         350       0.0000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00       NegIon         151       0.0000000E+00       0.0000000E+00       0.0000000E+00       NegIon         152       0.0000000E+00       0.0000000E+00       0.0000000E+00       NegIon         152       0.0000000E+00       0.0000000E+00       0.0000000E+00       NegIon         153       0.0000000E+00       0.0000000E+00       0.0000000E+00       NegIon         154       0.0000000E+00       0.0000000E+00       0.0000000E+00       Boron         155       0.0000000E+00       0.0000000E+00       0.0000000E+00       TracerEl         155       0.0000000E+00       0.0000000E+00       0.0000000E+00       Nc(III)         155       0.0000000E+00       0.0000000E+00       Nc(III)         155       0.0000000E+00       0.0000000E+00       Nc(III)         155       0.0000000E+00       0.0000000E+00       Nc(III)         155       0.00000000E+00       0.0000000E+00 </td <td></td>										
3-4       0.00000000000000000000000000000000000										
33.477768555±00       6.18147537E-03       5.534188642-03       6.64711398E+01       Carbon         D55       0.0000000E+00       0.0000000E+00       0.0000000E+00       Posion         C22       0.0000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00         C22       0.0000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00       Air         C22       0.0000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00       Boron         C23       0.0000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00       Boron         C45       0.0000000E+00       0.0000000E+00       0.0000000E+00       D.0000000E+00       TracerEl         C45       0.0000000E+00       0.0000000E+00       0.0000000E+00       D.0000000E+00       Ai(III)         C45       0.0000000E+00       0.0000000E+00       0.0000000E+00       U(VI)       TracerEl         C45       0.0000000E+00       0.0000000E+00       0.0000000E+00       U(VI)       TracerEl         C45       0.0000000E+00       0.0000000E+00       0.0000000E+00       U(VI)       TracerEl         C45       0.0000000E+00       0.0000000E+00       0.0000000E+00       D.00000000E+00       Fhosphorus										
D35       0.00000000000000000000000000000000000										
131       0.00000000000000000000000000000000000										
6122       0.00000000000000000000000000000000000	15 E									
625       0.00000000000000000000000000000000000	έź2 -									
0.00000000000000000000000000000000000	683									
0.00000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00       TracerEl         0.0000000E+00       0.0000000E+00       0.0000000E+00       TracerEl       TracerEl </td <td>34</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	34									
0.00000000000000000000000000000000000	055			0.0000000E+00						
0.00000000000000000000000000000000000										
2:1:0       3.47561578E+00       6.66349238E-06       5.96573175E-06       1.41416597E+00       Np(V)         2:8:0       0.0000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00       Clo4-(EL)         2:8:0       0.0000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00       Clo4-(EL)         2:0:0       0.0000000E+00       0.0000000E+00       0.0000000E+00       0.0000000E+00       Electron         2:0:0       -1.13087115E-15       -3.24368928E-15       -2.90402975E-15       0.0000000E+00       Charge         2:0:0       Solution Parameters, Calculated       -2.90402975E-15       0.0000000E+00       Charge         2:0:0       MASS       342.637323019311       grams       -2.90402975E-15       0.000000E+00         2:0:0       MASS       348.637323019311       grams       -2.90402975E-15       0.00000E+00         2:0:0       MASS       348.637323019311       grams										
0.00000000000000000000000000000000000										
0.00000000000000000000000000000000000										
0.00000000000000000000000000000000000										
3       -1.13087115E-15       -3.24368928E-15       -2.90402975E-15       0.0000000E+00       Charge         CCC       Solution Parameters, Calculated							•			
(24           CCC         Solution Parameters, Calculated           28*         SOLUTION MASS         462.933810446950         grams           28*         SOLUTION MASS         348.637323019311         grams           28*         TDS(g/kg)         327.837784084031         g/kgH20           28*         Specified Solution Density         1188.79464008680         kg/m^3 = g/l										
Solution Parameters, Calculated           Solution Parameters, Calculater, Calculater	(04									
SOLUTION MASS         462.93810446950         grams           OFD         H20 MASS         348.637323019311         grams           D55         TDS(g/kg)         327.837784084031         g/kg/20           UA         Specified Solution Density         57         DENSITY         1188.79464008680         kg/m^3 = g/1	CC2 -	Solution Paramete	rs, Calculated							
255 TDS(g/kg) 327.837784084031 g/kgH2O 125 070 Specified Solution Density 071 DENSITY 1188.79464008680 kg/m ⁻ 3 ≠ g/l	5.0	SOLUTION MASS	462.9338104469							
CCC Specified Solution Density CCC DENSITY 1188.79464008680 kg/m^3 = g/l	047			11 grams						
CCC Specified Solution Density CCC DENSITY 1188.79464008680 kg/m^3 = g/l	225	TDS (g/kg)	327.8377840840	31 g/kgH20						
07% DENSITY 1188.79464008680 kg/m ⁻ 3 ≅ g/l	1.74 1.74		. Desails							
		specified Solutio								
		TATAT CT THE	1100 704640000	ο <u>Λ</u> <u>ι_ ι_ Α</u> ··						

1073	Solution Parame	ters Based on Spec	cified Density						
1.274	SOLUTION VOL	0.389414449591 293.508593601	688 liters						
1075 1075									
	Density based of	on TDS and NaCl so we error vs NaCl do	lutions 1188.7 ensity 0.00000	9464008680 000000000E+000	g/l %				
1070					•				
()?) (3									
132	TABLE OF CONCENTR	ATIONS FOR BATCH :	SYSTEM						
:022 :022	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Decorintor
1023			-			socur noses	moldily	ng/ 11 Lei	Descriptor
	H2O NaNpO2CO3(s)	WATER NaNp02C03 (s)	8.31919E-01 9.96914E+00	7.78249E-01 1.00000E+00	0.9355 1.000	1.93524E+01 3.47561E+00	4.96961E+01 8.92523E+00	8.95286E+05	
133	Na+	Na+	5.61002E+00	5.28690E+00	0.9424	1.95586E+00	5.02257E+00	3.14209£+06 1.15468E+05	
1020	Cl-	C1-	5.59866E+00	5.27483E+00	0.9422	1.95190E+00	5.01240E+00	1.77705E+05	
	CO3+ HCO3-	C03= HC03-	5.06627E-03 1.09867E-03	1.31507E-04 4.06389E-04	2.5957E-02 0.3699	1.76629E-03 3.83037E-04	4.53576E-03 9.83623E-04	2.72187±+02 6.00178±+01	
1.00	OH-	OH-	1.01865E-04	5.54263E-05	0.5441	3.55141E-05	9.11987£-05	1.55104E+00	-1,77E-10
1003	NpO2 (CO3) 2=- NpO2 (CO3) 3==-	NpO2 (CO3)2=- NpO2 (CO3)3==-	3.23222E-06 3.29354E-06	8.41283E-11 2.65024E-15	2.6028E-05	1.12687E-06	2.89376E-06	1.12586E+00	8,12E-10
	CO2 (aq)	CO2 (aq)	5.53405E-08	1.60697E-07	8.0468E-10 2.904	1.14825E-06 1.92938E-08	2,94866£-06 4,95456£-08	1.32417E+00 2.18049E-03	1.75E-09 -9.24E-09
1.24	Np02C03~	Np02C03-	1.33806E-07	2.43236E-07	1.818	4.66498E-08	1,19795E-07	3.94192E-02	5.06E-13
1.37	NpO2+	NpO2+ H+	3.76324E-09 3.62550E-11	7.45944E-09 1.41496E-10	1.982 3.903	1.31200E-09	3,36917E-09	9.06465E-04	-7.98E-10
5	Np020H (aq)	NpO2OH(aq)	1.59617E-10	1.596176-10	1.000	1.26398E-11 5.56486E-11	3,24586E-11 1,42903£-10	3.27150E-08 4.08781E-05	-4.95E-09 4.15E-09
	Np02 (OH) 2-	Np02 (OH) 2-	1.42919E-12	4.26699E-13	0.2986	4.98268E-13	1,27953E-12	3.87777E-07	9.11E-09
112-1 112-2	Na3H(CO3)2.2H2O Na2CO3.H2O	Trona Thermonatrite	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1.000 1.000	0.00000E+00 0.00000E+00	0,00000E+00 0,00000E+00	0.00000E+00 0.00000E+00	-4.28E+00 -3.03E+00
1103	Na2CO3.7H20Na	2C03-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0,00000E+00	0.00000E+00	-2.74E+00
	Na2CO3.10H20	Natron		1.00000E+00	1.000	0.00000E+00	0,00000E+00	0.00000E+00	-2.70E+00
1106		Nahcolite Halite	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1.000 1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000£+00 0.00000£+00	-2.26E+00 -1.25E-01
::::::			0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.31E+02
	NaOH(aq)to.		0.00000E+00 0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.94E+02
	NpO20H(amor) NpO20H(aged)		0.00000E+00	1.00000E+00 1.00000E+00	1.000 1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-3.66E+00 -3.07E+00
1964			0.0000E+00	0.00000E+00	1.000	0.00000E+00	D.00000E+00	0.00000E+00	-2.49E+02
1952	pmH = -log[m(H+)]		= 10.4406						
1114	pH = -log[a(H+)]	= 9.8493	- 10.4400					•	
1115	Osmotic Coefficie								
1113	Equilibrium RH (% Ionic Strength (m								
1953		= 1188.79							
1114 1124	NOTES: - Water "	molality: is mole	fraction #20 in a	ameous phase					
1121		lality" and "activ							
1122		ptor means:							
1123 1124		ln10 for species w tion Index for min			criterion)				
112:	*logi0(	activity) for aque	ous species with		entrations				
1125	*log10()	partial pressure)	for gases						
	Total G/RT= -4	.64072873E+03							
	Flashing Titration								
	<pre># inversions for 1 1Benchmark TITRATE</pre>		ZZ DEION: ND(V)O2 with	th CO3 in 5.61mc	al NaCl F	MT V2.0			
1122	DATABASE: HMW84/	FW86; Np(V)-Na-CO3	-OH-C1-C104 (NR94	4);					
1133 1134	95.01.31 Am(III Pressure=	)-Na-C1-C03-S04-PC 1.00000E+00 [=] J			1,RRFF94} [=] Kelvin				
1135	F1635416-	1.000002+00 [-] 4	taperata	2.982402	[-] Keivin				
::20	Elemental Abundan	ces for Flash Prob	lem						
1127 1138	Total Moles	Aq. Molality	Ag. Molarity	Aq. mg/liter					
133									
1140 1141	3.87560135E+01	1.11018653E+02	9,93942650E+01	1.00179480E+05					
102	3.67651156E+01 5.43404174E+00	5.55352555E+01 5.61002728E+00	4.97203463E+01 5.02262026E+00	7.95495709E+09 1.15468885E+09					
1143	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	Potassium				
1144 1145	0.00000000E+00 0.00000000E+00	0.0000000E+00 0.0000000E+00	0.0000000E+00 0.0000000E+00	0.00000000E+00 0.00000000E+00				a start and a start and	
1.40	1.95263769E+00	5.59343408E+00	5.00776448E+00	1.77540274E+05					Sec. 2
1147	D.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	) Sulfur				
1948 1949	3.47868370±+00 0.00000000±+00	8.80060113E-03 0.00000000E+00	7.87911990E-03 0.00000000E+00	9.46361091E+01 0.00000000E+00					
1150	0.00000000E+00	0.0000000E+00	0.00000000E+00	0.00000000E+00				:	تكو
1151	0.00000000E+00	0.0000000E+00	0.0000000000000000000000000000000000000	0.0000000E+00					م . ج
1150 1153	0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00					1
1.154	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00	) TracerEl				
: ::	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00					
1158 1157	0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00	0.0000000E+00 0.0000000E+00	0.0000000E+00 0.0000000E+00					
1.55	3.47561578E+00	1.23872216E-05	1.10901974E-05	2.62891134E+00					
**55 - 160	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00		_			
1.61	0.00000000E+00 0.00000000E+00	0.0000000CE+00 0.0000000CE+00	0.00000000E+00 0.00000000E+00	0.0000000E+00	-	•			
11£2	-6.72313767E-16	-1.92587840E-15	-1.72422617E-15	0.0000000E+00					

Some day in the

1153									
1.54	Solution Parame	ters, Calculated							
	SOLUTION MASS		54 grams						
110	H20 MASS	349.0946099546							
1:57	TDS(g/kg)	327.8123629139	-						
1.1.1			÷ -						
11.2	Specified Solut	ion Density							
	DENSITY	1188.781612593	127 kg/m^3 =	g/l					
• • • • •									
	Solution Parame	ters Based on Spec	ified Density						
. 71	SOLUTION VOL	0.3899220294241	.27 liters						
<u> </u>	TDS	293.4882369656	187 g/l						
	·								
· • · · ;	Density based of	n TDS and NaCl sol		8161259327	g/l				
1 i r r	Percent relative	e error vs NaCl de	msity 0.00000	00000000000E+000	*				
:72 -7									
1122									
• • • •	TABLE OF CONCENTR	ATIONS FOR BATCH S	W CTUREM						
- 150	THELE OF CONCENTIO		101121						
	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
190							northrity	ng/licer	Descriptor
	H20	WATER	8.31951E-01	7.78350E-01	0.9356	1.93778E+01	4.96966E+01	8.95293E+05	
	NaNp02C03(s)	NaNpO2CO3(s)	9.95607E+00	1.00000E+00	1.000	3.47561E+00	8.91361E+00	3.13800E+06	
1987	Na+	Na+	5.61003£+00	5.28539E+00	0.9421	1.95843E+00	5.02262E+00	1.15469E+05	
1150	C1-	C1-	5.59343E+00	5.26704E+00	0.9416	1.95264E+00	5.00776E+00	1.77540E+05	
1.134	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	€.24350E+01	
1.51	OH-	OH-	1.47379E-04	8.02242E-05	0.5443	5.14493E~05	1.31948E-04	2.24408E+00	-2.23E-08
	Np02(C03)2=-	Np02 (C03) 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==-	7.39875E-06	6.00222E-15	8.1125E-10	2.58286E-06	6.62405E-06	2.97469E+00	3.56E-08
	CO2 (aq) NpO2CO3 -	CO2 (aq)	3.97510E-08	1.15435E-07	2.904	1.38769E-08	3.55888E-08	1.56626E-03	-3.82E-07
		NpO2CO3-	1.33905E-07	2.43306E-07	1.817 1.978	4.67454E-08	1.19884E-07	3.94486E-02	2.95E-11
197	NpO2+	NpO2+ H+	2.50641E-09 2.51081E-11	4.95882E-09 9.77709E-11	3.894	8.74975E-10 8.76512E-12	2.24398E-09	€.03735E-04	-1.78E-08
	NpO2OH(aq)	NpO2OH(ag)	1.53583E-10	1.53583E-10	1.000	5.36149E-11	2.24792E-11 1.37502E-10	2.26567E-08 3.93329E-05	-1.28E-07 1.10E-07
	Np02 (OH) 2-	Np02 (OH) 2-	1.99131E-12	5.94256E-13	0.2984	6.95155E-13	1.78281E-12	5.40300E-07	2.38E-07
1001	Na3H(CO3)2.2H20	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	C.00000E+00	-4.08E+00
	Na2C03.H20	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	C.00000E+00	-2.85E+00
2.2		2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	C.00000E+00	-2.56E+00
202	Na2CO3.10H20	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	C.00000E+00	-2.52E+00
1.1.1		Nahcolite	0.0000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	C.00000E+00	-2.25E+00
	NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	C.00000E+00	-1.26E-01
	Na3Np02(C03)2(s)_1		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	C.00000E+00	-9.31E+02
119	NaOH(ag)to.t		0.00000E+00 0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	C.00000E+00	-2.94E+02
	NpO20H(amor) NpO20H(aged)		0.00000E+00	1.00000E+00 1.00000E+00	1.000	C.00000E+00 C.000C0E+00	0.000002+00	C.00000E+00	-3.68E+00
- 312			0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00 0.00000E+00	C.00000E+00 C.00000E+00	-3.09E+00 -2.49E+02
- 211							0.000000.00	0.0000000000	-2.432+02
211	pmH = -log[m(H+)]		= 10.6002						
	$pH = -log[a{H+}]$	= 10.0098							
	Osmotic Coefficier								
1215	Equilibrium RH (%)								
1212	Ionic Strength (m)								
	Density, kg/m3	= 1188.78							
	NOTES: - Water "m	nolality' is mole	fraction H2O in a	noueous phase					
:220		lality and activ							Sector of Contraction
:22 :	- "Descrip	otor means:							, <b>*</b>
:222	•dG/RT/]	in10 for species w	ith nonzero conce	s. {convergence	criterion)				
1,23		tion Index for min						,	· ·
		ectivity) for aque		very small con	centrations				
22	*log10(p	partial pressure)	IOT GASES						
220	Total G/RT= -4.	64367246E+03							
	Flashing Titration								
	t inversions for b		22						
(25)	lBenchmark TITRATE	Problem, LOG10 op	tion; Np(V)02 wit	th CO3 in \$.61m	olal NaCl - H	MT V2.0			
۰.	DATABASE: HMW84/F								
		-Na-C1-C03-S04-P0							
233	Pressure=	1.00000E+00 [=] A	TM Temperatur	re= 2.98£+0	2 [=] Kelvin				
	Elemental Abundanc	es for Flach Prob	lem						
1055									
13 32	Total Moles	Ag Molality	Ag. Molarity	Aq. mg/liter					
12.2.2									•
2.	3.88284068E+01	1.11018771E+02	9.93954996E+01	1.00180724E+0					
- 240	3.68052248E+01	5.55465070E+01	4.97309848E+01	7.95665918E+0					
1.2.1	5.43769997E+00	5.61004415E+00	5.02269243E+00	1.15470544E+0					
4	0.0000000E+00	0.0000000E+00	0.0000000£+00	0.0000000E+0					
12.40	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+0	•				
246	0.00000000E+00	0.00000000E+00 5.58601315E+00	0.00000000E+00	0.00000000E+0					
120	1.95368755E+00 0.0000000E+00	5.58601315E+00 0.00000000E+00	5.00117739E+00 0.00000000E+00	1.77306742E+0 0.00000000E+0					
24.	3.47998788E+00	1.25239828E-02	1.12127662E-02	1.34676535E+0					
243	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.0000000E+0					
្នើនទ្	0.0000000E+00	0.00000000E+00	0.0000000E+00	0.00000000E+0					
12.50	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+0	-				
20	0.0000000E+00	0.0000000E+00	0.00000000E+00	0.0000000E+0					
252	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+0					

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

1993 1994 1994 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 TracerE1 0.0000000E+00 0.00000000±+00 0.0000000E+00 0.0000000E+00 Th(IV) 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Am(III) 2.60 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 U(VI) 3.47561578E+00 2.32128943E-05 2.07825866E-05 4.92647476E+00 Np(V) 2.7 C104-(EL) 0.00000002+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 1.53 Phosphorus 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000±+00 0 00000000E+00 0.0000000E+00 D.0000000E+00 0.0000000E+00 Electron -8.43194194E-16 -2.41087366E-15 -2.15846374E-15 0.00000000E+00 Charge 100 Solution Parameters, Calculated 464.385150217386 349.746321818902 SOLUTION MASS GTARS H2O MASS grams 327.777080834729 TDS(g/kg) a/kaH20 Specified Solution Density 280 1188.76353136245 kg/m^3 ≖ g/l DENSITY Solution Parameters Based on Specified Density 0.390645521977908 SOLUTION VOL liters 293.459983409119 TDS a/1 :2.76 294 1971 Density based on TDS and NaCl solutions 1188.76353136245 g/1 Percent relative error vs NaCl density 0.00000000000000E+000 % 114 12.31 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM .2.÷ 1202 Species Name 1353 Molality Activity Act Coef Total Moles Molarity mg/liter Descriptor -H20 WATER 8.31997E-01 7.78493E-01 0.9357 1.94140E+01 4.96971E+01 8.95304E+05 125 NaNp02C03(s)_ NaNp02003 (5) 9.93751E+00 1.00000E+00 1.000 3.47561E+00 8.89709E+00 3.13218E+06 1230 Na+ 5.61004E+00 5.28333E+00 0.9418 Na+ 1.96209E+00 5.02269E+00 1.15471E+05 1267 C1-¢1-5.58601E+00 5.25591E+00 0.9409 1.95369E+00 5.00118E+00 1.77307E+05 1222 CO3= **003**≢ 1 12609E-02 2 92079E+04 2 59378-02 3.93846E-03 1.00819E-02 6.05009E+02 1.00 HC03-1.20082E-03 4.43607E-04 нсоз-0.3694 4.19981E-04 1.07510E-03 6.55992E+01 🗆 : ) он-OH-2.07123E-04 1.12810E-04 0.5447 7.24404E-05 1.85438E-04 3.15380E+00 -2.25E-09 Np02(C03)2=~ 12.521 NDO2(CO3)2 = -7.13717E-06 1.86975E-10 2.6197E-05 2.49620E-06 6.38993E-06 2,48610E+00 4.21E-09 1.52 NDO2 (CO3) 3==-1.30821E-14 Np02(C03)3##-1.59398E-05 8.2072E-10 5.57490E-06 1 427105-05 6 40874E+00 8.72E-09 2.8 CO2 (ag) CO2 (ag) 2.96765E-08 8.61856E-08 2.904 1.03792E-08 2.65695E-08 1.16932E-03 -9.22E-08 1.34044E-07 1.70329E-09 2.43401E-07 · ) 4 Np02C03-Np02C03-1.816 4.68815E-08 1.20010E-07 3.94902E-02 8.14E-12 1936 Np02+ 1955 Np020H(ag) 1257 H+ Np02+ 3.36086E-09 1.973 5.95718E-10 1 524965-09 4.10285E-04 -4.25E-09 NpO2OH (ag) 1.46370E-10 1.46370E-10 1.000 5.11925E-11 3.74863E-05 1.31046E-10 4.11E-08 H+ 1.79163E+11 6.95424E-11 3.882 6.26615E-12 1.60405E-11 1.61672E-08 -4.53E-08 1283 Np02 (OH) 2-ND02 (OH) 2-2.67040E-12 7.96388E-13 0.2982 9.33963E-13 2.39082E+12 7.24565E-07 8.64E-08 1203 Na3H(CO3)2.2H20 1203 Na2CO3.H20 Trona 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -3.89E+00 Thermonatrite 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.68E+00 Na2CO3-Heptahydrate 001 Na2CO3.7H2O 1.00000E+00 -2.39E+00 0.00000±+00 1,000 0.00000E+00 0.00000E+00 0.00000E+00 Na2C03.10H20 Natron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.35E+00 iaca retk NaHCO3_ Nahcolire 0.000005+00 1.00000E+00 1.000 0.00000£+00 0.00000E+00 0.00000±+00 -2.23E+00 NaCl. 0.00000E+00 1.00000E+00 Halite 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 0.0000E+00 0.00000£+00 0.00000E+00 -9.31E+02 · . , , 1.000 NaOH(aq)....to.titrate.base.only 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 -2.94E+02 NpO2OH(amor)_____ NpO2OH(aged)____ Np020H(amor) 1.00000E+00 0.00000E+00 1,000 0.00000E+00 0.00000E+00 0 000008+00 -3.70E+00 _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 0.0000000+00 0.00000E+00 1 000 0.0000E+00 0.00000E+00 0.00000E+00 -2.50E+02 1211  $pmH = -\log[m(H+)]$ 10.7468 pH = -log[a(H+)]= 10.1578 1318 Osmotic Coefficient= 1.240021 1314 Equilibrium RH (%) * 77.849336 14:1 Ionic Strength (m) = 5.621486 Sec Density, kg/m3 1188.76  $1238^\circ$  NOTES: - Water "molality" is mole fraction H2O in aqueous phase - Gas 'molality' and 'activity' are gas partial pressures 1210 1309 1351 - "Descriptor" means: *dG/RT/ln10 for species with nonzero concs. {convergence criterion} *Saturation Index for minerals, SI=log10(IAP/Ksp) :322 :225 *log10(activity) for aqueous species with very small concentrations *log10(partial pressure) for gases 327 151.5 195.2 Total G/RT= -4.64786705E+03 Flashing Titration # 12 323 # inversions for batch pblm 22 .620 IBenchmark TITRATE Problem, LOGIO option; Np(V)02 with CO3 in 5.61molal NaCl - FMT V2.0 DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-C1-C1O4 (NR94); 95.01.31 Am(III)-Na-C1-CO3-SO4-PO4 (FRSR89, FRF90, P91, RFFR92, RFF94, RRFF94) 12.20 1331 1330 1.00000E+00 [#] ATM 2.98£+02 [=] Kelvin Pressure= Temperature* 323 :25/ Elemental Abundances for Flash Problem :251 Total Moles Ac. Molality Ag. Molarity Aq. mg/liter 1337 1.00182423E+05 Hydrogen ుసా 3.89315747E+01 1.11018923E+02 9,93971848E+01 :335 3.68623846E+01 5.55624877E+01 4.97460679±+01 7.95907238E+05 Oxygen 210 5.61007250E+00 5.02279611E+00 5.44291331E+00 1.15472927E+05 Sodium 126. 0.0000000E+00 0.00000000±+00 0.00000000E+00 Potassium 13.2 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Magnesium

πg/liter

£.95318E+05 3.12393E+06 1.15473E+05 1.76975£+05 8.81956E+02 6.96709E+01 4.32833E+00

3.60399E+00 1.33836E+01 9.03107E-04

3.95491E-02 2.82874E-04 3.53631E-05 1.18280E-08 5.39711E-07

(.00000E+00

C.00000E+00 (.00000E+00 C.00000E+00 C.00000E+00 (.00000E+00

C.00000E+00 C.00000E+00

(.00000E+00 (.00000E+00

Descriptor

-1.42E-09 2.42E-09 5.14E-09 -7.40E-08

6.18E-12 -2.46E-09 3.39E-08

-3.64E-08 7.04E-08

-3.70E+00

-2.52E+00 -2.23E+00 -2.19E+00 -2.20E+00 -1.28E-01

-9.30E+02

-2.94E+02 -3.73E+00

-3.13E+00 -2.50E+02

and the second sec

-	Appendix N: Sai	nple Output File	"Np_NaCl_BM	A_LOG.OUT"			
			-				
1242	0.0000000E+00		0.0000000£+00	0.0000000£+0	) Calcium		
1344	1.95518372E+00	5.57548446E+00	4.99182884E+00	1.76975308E+0	5 Chlorine		
111	0.00000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+0	0 Sulfur		
245	3.48184647E+00		1.59469162 <b>2-0</b> 2	1.91538411E+0			
1.7	0.00000000E+00		0.0000000E+00	0.00000000E+0			
			0.00000000E+00	0.00000000E+0			
.2`	0.0000000E+00						
14 3 1	0.0000000E+00		0.0000000E+00	0.0000000E+0			
33-3	0.0000000E+00		0.0000000E+00	0.0000000E+0			
	0.000000000000000	0.0000000E+00	0.0000000E+00	0.0000000E+0	) Bromine		
1.2	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+0	D TracerEl		
282	0.0000000E+00	0.0000000E+00	0.0000000E+00	D.0000000E+0	0 Th(IV)		
24.2	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+0	Am(III)		
266	0.0000000E+00		0.0000000E+00	0.0000000E+0			
28 -	3.47561578E+00		3.91872342E-05	9.28926332±+0			
952			0.0000000E+00	0.00000000E+0			
203	0.0000000E+00		0.00000000E+00				
	0.0000000E+00		0.00000000E+00	0.0000000E+0 0.00000000E+0			
	0.000000000000000						
	-1.32033463E-15	-3.76512199E-15 -	3.3/09/9625-13	0.0000000E+0	J Charge		
		<b>6</b> · 1 · · 1 · · · · · · · · · · · · · ·					
220	Solution Paramet		_				
350	SOLUTION MASS	465.60142060626	-				
1.4	H20 MASS	350.67512635209	6 grams				
. :	TDS(g/kg)	327.72867425670	0 g/kgH2O				
ΞŤ.							
(-2 TV	Specified Soluti	on Density					
5.25	DENSITY	1188.7387234679	4 kg/m^3 =	g/l			
55				• -			
	Solution Paramet	ers Based on Speci	fied Density				
2	SOLUTION VOL	0.39167683479508					
••••		293.42121883286					
	TDS	233.44141003400	~ 9/±				
375					- (7		
24		TDS and NaCl solu		3872346794	g/1		
575	Percent relative	error vs NaCl den	sity 0.00000	0000000000E+000	5		
37C							
677							
172							
377 Q	TABLE OF CONCENTRA	TIONS FOR BATCH SY	STEM				
50 C.S.C							
	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity
332							
383	H20	WATER	8.32061E-01	7.78697E-01	0.9359	1.94655E+01	4.96979E+01
	NaNp02C03(s)	NaNp02C03(s)	9.91117E+00	1.00000E+00	1.000	3.47560E+00	8.87364E+00
				5.28057E+00	0.9413	1.96731E+00	
25		Na+	5.61007E+00				5.02280E+00
256		C1-	5.57548E+00	5.24002E+00	0.9398	1.95518E+00	4.99183E+00
	C03=	CO3=	1,64154E-02	4.25480E-04	2.5920E-02	5.75648E-03	1.46970E-02
8.2	HCO3-	нсоз-	1.27533E-03	4.70618E-04	0.3690	4.47227E-04	1.14183E-03
74		OH-	2.84255E-04	1.54942E-04	0.5451	9.96812E-05	2.54499E-04
	NpO2 (CO3) 2=-	Np02 (C03) 2=~	1.03463E-05	2.72515E-10	2.6339E-05	3.62818E-06	9.26320E-06
	NpO2 (CO3)3==-	NpO2 (CO3) 3==-	3.32873E-05	2.77756E-14	8.3442E-10	1.16730E-05	2.98027E-05
	C02(ag)	CO2 (ag)	2.29199E-08	6.65707E-08	2.904	8.03744E-09	2.05206E-08
	NpO2CO3-	Np02C03-	1.34242E-07	2.435282-07	1.814	4.70755E-08	1.20190E-07
	NpO2+	NpO2+	1.17432E-09	2.30833E-09	1.966	4.11805E-10	1.05139E-09
		NpO20H(ag)		1.38078E-10	1.000		
	NpO2OH(aq)		1.38078E-10			4.84205E-11	1.23624E-10
32		H+	1.31074E-11	5.06455E-11	3.864	4.59643E-12	1.17353E-11
	NpO2(OH)2-	NpO2 (OH) 2-	3.46327E-12	1.03185E-12	0.2979	1.21448E-12	3.10073E-12
	Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.0000CE+00	0.0000E+00
	Na2CO3.H20	Thermonatrite	0.00000£+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00
00	Na2CO3.7H20Na2	CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00
	Na2CO3.10H20	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00
	NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00
	NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00
	Na3NpO2(CO3)2(s)_L		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00
	NaOH(ag) to.t	itrate hase only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00
	NpO2OH(amor)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	
				1.00000E+00			
	NpO2OH(aged)		0.00000E+00		1.000	0.00000E+00	
	HCl(ag)to.t	itrate.acid.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00
:03							
10	pmH = -log[m(H+)]	2	10.8825				
		= 10.2955					
	Osmotic Coefficier	t= 1.239297					
33	Equilibrium RH (%)	= 77.869707					
	Ionic Strength (m)						
	Density, kg/m3						
115							
	NOTES: - Water ""	colality is mole for	raction H2O in a	aqueous phase			
(13) (13)		ality and activi					
			el are dar hau	rigi hissonsi			
( 1 <u>6</u> .	-	tor means:		- /			
-20		n10 for species wi			criterion)		
1		ion Index for mine					
		ctivity) for aqueo		very small con	centrations		
	*log10(p	artial pressure) fo	or gases				
5 C C							
-23	Total G/RT= -4.	65384406E+03					
	Flashing Titration						
. 7	# inversions for b	atch pblm	22				
		Problem, LOG10 opt.		th CO3 in 5.61m	lal NaCl F	MT V2.0	
		W86; Np(V)-Na-CO3-			••••••		
		-Na-C1-C03-S04-P04			RRFF941		
				rsi,krrks2,krrs re≠ 2.98£+0			
	Pressure=	1.00000E+00 [=] AT	n iemperatui	LC- 4.302+U	- [-] vetviu		
e							

.....

.

mg/liter

8.95336E+05

3.11224E+06 1.15476E+05 1.76506E+05

1.76506E+05 1.27367E+03 7.48201E+01 5.81986E+00 5.16313E+00

2.72222E+01 7.19279E-04

7.19279E-04 3.96323E-02 1.97283E-04 3.30183E-05 8.84779E-09

C.04772-055-06 C.00000E+00 C.00000E+00 C.00000E+00 O.00000E+00 O.00000E+00 O.00000E+00 O.00000E+00 D.00000E+00 D.00000E+00 Descriptor

-1.17E-09 1.59E-09 3.46E-09 -6.83E-08 5.31E-12

5.31E-12 -1.64E-09 3.16E-08 6.48E-08 -3.32E-08 6.48E-08 -2.35E+00 -2.07E+00 -2.07E+00 -2.17E+00 -1.31E-01 -9.30E+02 -3.76E+00 -3.16E+00 -2.50E+02

	Elemental Abundan	ces for Flash Prob	lem				
1434 1435	Total Moles	Ag. Molality	Ag. Molarity	Ag. mg/liter			
130							
1437	3.90785996E+01	1.11019115E+02	9.93994493E+01	1.00184705E+05			
	3.69438430E+01	5.55851538E+01	4.97674088E+01	7.96248680E+05			
1433 1440	5.45034287£+00	5.61012129E+00 0.00000000E+00	5.02294553±+00 0.0000000±+00	1.15476363E+05 0.00000000E+00			
:44	0.00000002+00 0.00000002+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			
142	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			
1.00	1.95731591E+00	5.56057489E+00	4.97858483E+00	1.76505768E+05			
*	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00			
1440	3.48449515E+00	2.53082323E-02	2.26593804E-02	2.72161818E+02	Carbon		
144.5	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00			
1447	0.0000000E+00	C.00000000E+00 0.00000000E+00	0.0000000E+00	0.00000000E+00 0.00000000E+00			
- 288 - 285	0.0000000E+00 0.0000000E+00	0.0000000E+00	0.00000000E+00 0.0000000E+00	0.00000000E+00			
1450	0.00000000E+00	0.0000000E+00	0.00000000E+00	0.00000000E+00			
1451	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00			
14-51	0.0000000E+00	0.000000000000+00	0.0000000E+00	0.0000000E+00	Th(IV)		
1463	0.0000000E+00	0.00000000E+00	0.0000000£+00	0.0000000000000000000000000000000000000			
1484	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00			
	3.47561578E+00	8.26620364E-05	7.40103261E-05	1.75440146E+01	-		
1498 1437	0.0000000E+00 0.0000000E+00	0,0000000E+00 0.0000000E+00	0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00			
1455	0.00000000E+00	0.0000000E+00	0.00000000E+00	0.00000000E+00	-		
:459	-1.25055944E-15		-3,18089495E-15	0.0000000E+00			
-⊀£(							
1481		ters, Calculated					
1462	SOLUTION MASS	467.3359434300	-				
1423 1995	H2O MASS TDS(g/kg)	351.9988396874 327.6633066318	-				
1444	103(3/23)	527.005500020	<b>y</b> , y,				
14CC	Specified Solut:	ion Density					
:<27	DENSITY	1188.705221976	51 kg/m^3 =	g/l			
- 52							
1453		ters Based on Spec					
147) 1471	SOLUTION VOL TDS	0.3931470433460 293.3688697260					
1472	100	1991100009/100					
.472	Density based of	n TDS and NaCl sol	utions 1188.70	522197651	g/l		
1474	Percent relativ	e error vs NaCl de	nsity 0.000000	0000000000E+000	8		
1475							
1475 1472							
	TABLE OF CONCENTRA						
			ISTER				
1670		MILONS FOR BAICS 3	ISIDA				
1470 1420	Species Name	ALIONS FOR BAILS 3	Molality	Activity	Act Coef	Total Moles	Molarity
1470 1420 1431	Species Name		Molality	-			-
1499 1480 1481 1481	Species Name H20	WATER	Molality 8.32153E-01	7.78985E-01	0.9361	1.95390E+01	4.96989E+01
1478 1480 1481 1451 1452 1452	Species Name H20 NaMpO2CO3(s)	WATER NaNpO2CO3(s)	Molality 8.32153E-01 9.87386E+00	7.78985E-01 1.00000E+00	0.9361 1.000	1.95390E+01 3.47559E+00	4.96989E+01 8.84042E+00
1499 1480 1481 1481	Species Name H2O NaMpO2CO3(s) Na+	WATER	Molality 8.32153E-01	7.78985E-01 1.00000E+00 5.27693E+00	0.9361	1.95390E+01	4.96989E+01
1490 1480 1481 1482 1483 1483 1483	Species Name H2O NaMpO2CO3(s) Na+	WATER NaNpO2CO3(s) Na+	Molality 8.32153E-01 9.87386E+00 5.61012E+00	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00	0.9361 1.000 0.9406	1.95390E+01 3.47559E+00 1.97476E+00	4.96989E+01 8.84042E+00 5.02295E+00
1470 1480 1485 1485 1488 1488 1488 1488 1488 1488	Species Name H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3-	WATER NaNpO2CO3(s) Na+ Cl- CO3= HCO3-	Molality 8.32153E-01 9.87386E+00 5.61012E+00 5.56057E+00 2.37058E-02 1.36956E-03	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 5.04583E-04	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684	1.95390E+01 3.47559E+00 1.97476E+00 1.95732E+00 8.34440E-03 4.82083E-04	4.96989E+01 8.84042E+00 5.02295E+00 4.9785E+00 2.12246E-02 1.22622E-03
147901 147901 147902 147902 147902 147902 147902 147902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14902 14900 14902 14902 14902 14902 14902 14900 14900 14900 1490	Species Name H20 NaNpO2CO3(s) Na+ C1- C03= HCO3- OH-	WATER NaNpO2CO3(s) Na+ C1- CO3= HCO3- OK-	Molality 8.32153E-01 9.87366E+00 5.61012E+00 5.56057E+00 2.37058E-02 1.36956E-03 3.82200E-04	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 5.04583E-04 2.08552E-04	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457	1.95390E+01 3.47559E+00 1.97476E+00 1.95732E+00 8.34440E-03 4.82083E-04 1.34534E-04	4.96989E+01 8.84042E+00 5.02295E+00 4.97858E+00 2.12246E-02 1.22622E-03 3.42198E-04
10011000000000000000000000000000000000	Species Name H20 NaNpO2CO3(s) Na+ C1- C03= HCO3- OH- NpO2(CO3)2=-	WATER NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=-	Molality 8.32153E-01 9.87386E+00 5.56057E+00 2.37058E-02 1.36556E-03 3.8220E-04 1.48219E-05	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 5.04583E-04 2.08552E-04 3.93404E-10	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 4.82683E-04 1.34534E-04 5.21729E-06	4.96989E+01 8.84042E+00 5.02295E+00 4.97858E+00 2.12246E-02 1.2262E-03 3.42198E-04 1.32706E-05
1479011448852 14435528448867 14488848867 1448888867 144888888 144888888 14488888888 14488888888	Species Name H20 NaMp02C03(s) Na+ C1- C03= HC03- OH- Np02(C03)2=- Np02(C03)3==-	WATER NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==-	Molality 8.32153E-01 9.87386E+00 5.61012E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 5.04583E-04 2.08552E-04 3.93404E-10 5.78442E-14	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457	1.95390E+01 3.47559E+00 1.97476E+00 1.95732E+00 8.34440E-03 4.82083E-04 1.34534E-04	4.96989E+01 8.84042E+00 5.02295E+00 4.97858E+00 2.12246E-02 1.22622E-03 3.42198E-04 1.32706E-05 6.06184E-05
47501 14351 14352 14352 14352 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 14355 143555 143555 143555 1435555 143555 143555 143555 143555 143555 143555 1435555 1435555 1435555 14355555 14355555 1435555555555	Species Name H20 NaMp02C03(s) Na+ C1- C03= HC03- OH- Np02(C03)2=- Np02(C03)3==-	WATER NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=-	Molality 8.32153E-01 9.87386E+00 5.56057E+00 2.37058E-02 1.36556E-03 3.8220E-04 1.48219E-05	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 5.04583E-04 2.08552E-04 3.93404E-10	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 4.82083E-04 1.34534E-04 5.21729E-06 2.38320E-05	4.96989E+01 8.84042E+00 5.02295E+00 4.97858E+00 2.12246E-02 1.2262E-03 3.42198E-04 1.32706E-05
10111111111111111111111111111111111111	Species Name H20 NaMpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2+	WATER NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3-	Molality 8.32153E-01 9.87386E+00 5.56057E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10	7.78985E-01 1.0000E+00 5.27693E+00 5.21732E+00 6.13801E-04 5.04583E-04 2.06552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955	1.95390E+01 3.47559E+00 1.97476E+00 8.3440E-03 4.82083E-04 1.34534E-04 5.21729E-06 2.38320E-05 6.42544E-09 4.73516E-08 2.88282E-10	4.96989E+01 8.84042E+00 5.02295E+00 4.97858E+00 1.2262E-03 3.42198E-04 1.32706E+05 6.06184E-05 1.63436E+08 1.20442E+07 7.33267E+10
10111111111111111111111111111111111111	Species Name H20 Nah02C03(s) Na+ C1- C03= HC03- OH- Np02(C03)3==- C02(aq) Np02C03- Np02C3- Np02C3- Np02C4(aq)	WATER NaNpO2CO3 (s) Na+ C1- CO3= HCO3- 0H- NpO2 (CO3) 2=- NpO2 (CO3) 3=- CO2 (aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND3- ND	Molality 8.32153E-01 9.87366E+00 5.61012E+00 2.37058E-02 1.36556E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.1896E-10 1.28920E-10	7.78985E-01 1.0000E+00 5.27693E+00 5.21732E+00 6.13801E-04 5.04583E-04 2.08552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.28920E-10	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.000	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 4.82083E-04 1.34534E-04 3.34534E-04 2.38220E-05 6.42544E-09 4.73516E-08 2.88282E+10 4.53797E-11	4.96989±01 8.84042±00 5.02295±00 4.97858±00 2.12246E-02 1.22622±-03 3.42198E-04 1.32706E-05 6.06184±-05 1.63436E-08 1.20442E-07 7.33267E-10
11111111111111111111111111111111111111	Species Name H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=x- CO2(aq) NpO2CO3- NpO2+ NpO2OH(aq) H+	WATER NaNpO2CO3 (s) Na+ C1- CO3= HCO3- OH- NpO2 (CO3) 2=- NpO2 (CO3) 3=- CO2 (aq) NpO2CO3- NpO2CH (aq) NpO2CH (aq) H+	Molality 8.32153E-01 9.87386E+00 5.61012E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10 1.28920E-10 9.80463E-12	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 2.08552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.26920E-10 3.76405E-11	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.000 3.839	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 8.8208E-04 1.34534E-04 5.21729E-06 6.42544E-09 4.73516E-08 2.88282E+10 4.53797E-11 3.45122E-12	4.96989±01 8.84042±00 5.02295±00 4.97858±00 2.12246E-02 1.2262E-03 3.42198E-04 1.32706±-05 6.06184E-05 1.63436±-08 1.20442E-07 7.33267±-10 1.15427±-10 8.77844E-12
10111111111111111111111111111111111111	Species Name H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2(CO3- NpO2+ NpO2CH(aq) H+ NpO2(OH)2-	WATER NaNpO2CO3 (s) Na+ Cl- CO3= HCO3- OH- NpO2 (CO3) 2=- CO2 (aq) NpO2(CO3 (3=- CO2 (aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3- NpO3-	Molality 8.32153E-01 9.87366E+00 5.61012E+00 2.37058E-02 1.36556E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.1896E-10 1.28920E-10	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 2.08552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.26920E-10 3.76405E-11	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.000	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 4.82083E-04 1.34534E-04 3.34534E-04 2.38220E-05 6.42544E-09 4.73516E-08 2.88282E+10 4.53797E-11	4.96989±+01 8.84042±+00 5.02295±+00 4.97858±+00 1.22622±-03 3.42198±-04 1.32706±+05 1.63436±+08 1.20442±+07 7.33267±+10 1.154272±+10 8.77844±+12 3.90234±+12
	Species Name H20 NahpO2CO3(s) Na+ C1- C03= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3(CO3)2=- NpO3	WATER NaNpO2CO3 (s) Na+ C1- CO3= HCO3- OH- NpO2 (CO3) 2=- NpO2 (CO3) 3=- CO2 (aq) NpO2CO3- NpO2CH (aq) NpO2CH (aq) H+	Molality 8.32153E-01 9.87386E+00 5.56057E+00 2.37058E-02 1.36956E-03 3.8220E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10 1.28920E-10 9.80463E-12 4.35852E-12	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 2.08552E-04 3.93404E-10 5.75442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.28920E-10 3.76405E-11 1.29676E-12 1.00000E+00	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.800 3.839 0.2975 1.000 1.000	1.95390E+01 3.47559E+00 1.97476E+00 8.3440E-03 4.82083E-04 1.34534E-04 5.21729E-06 2.38320E-05 6.42544E-09 4.73516E-08 2.88282E-10 4.53797E-11 3.45122E-12	4.96989±01 8.84042±00 5.02295±00 4.97858±00 2.12246E-02 1.2262E-03 3.42198E-04 1.32706±-05 6.06184E-05 1.63436±-08 1.20442E-07 7.33267±-10 1.15427±-10 8.77844E-12
507101111111111111111111111111111111111	Species Name H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(ag) NpO2(CO3- NpO2+ NpO2CO3- NpO2+ NpO2(OH)2- Na2CO3.H20Na	WATER NaNp02CC03 (s) Na+ C03= HC03- OH- Np02 (CO3) 2=- C02 (aq) Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np02CO3- Np03- Np03- Np03- Np03- Np03- Np03- Np03- Np03- Np03- N	Molality 8.32153E-01 9.87386E+00 5.56057E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10 1.28926E-10 9.80463E-12 4.35852E-12 0.0000E+00 0.0000E+00 0.0000E+00	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 2.06552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.28920E-10 3.76405E-11 1.29676E-12 1.00000E+00 1.00000E+00	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.000 3.839 0.2975 1.000 1.000	1.95390E+01 3.47559E+00 1.97476E+00 8.3440E-03 4.82083E-04 1.34534E-04 5.21729E-06 2.38320E-05 6.42544E-09 4.73516E-08 2.88282E-10 4.53797E-11 3.45122E-12 1.53420E-12 0.0000E+00 0.0000E+00	4.96989±01 8.84042±00 5.02295±00 4.97858±00 1.22622=03 3.42198=04 1.32706±05 1.63436±08 1.20442±07 7.33267±10 1.154272±10 8.77844±-12 3.90234±-12 0.00000±00 0.00000±00
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Species Name H20 Nah02C03(s) Na+ C1- C03= HC03- OH- NpO2(C03)3=- C02(aq) NpO2C03- NpO2C3- NpO2C4(aq) H+ NpO2OH(aq) H+ NpO2OH(2- Na3H(C03)2.2H20Na Na2C03.10H20Na	WATER NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)3=- NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NPO3- NP	Molality 8.32153E-01 9.87366E+00 5.56057E+00 2.37058E-02 1.36556E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.1896E-10 9.80463E-12 4.3552E-12 0.00000E+00 0.00000E+00 0.00000E+00	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 2.08552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-09 1.28920E-10 3.76405E-11 1.29676E-12 1.00000E+00 1.00000E+00 1.00000E+00	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.905 1.000 3.839 0.2975 1.000 1.000 1.000	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 4.82083E-04 1.34534E-04 5.21729E-06 2.38320E-05 6.42544E-09 4.73516E-08 4.53797E-11 3.45122E-12 0.53420E-12 0.00000E+00 0.00000E+00	4.96983±01 8.84042±00 5.02295±00 4.97858±00 2.12246±-02 1.22622±-03 3.42198±-04 1.32706±-05 6.06184±-05 1.63436±-05 1.63436±-05 1.63436±-07 7.33267±10 1.15427±-10 8.77844±-12 3.90234±-12 0.00000±+00 0.00000±+00
10101111111111111111111111111111111111	Species Name H20 NaHpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2(OH)2- Na3H(CO3)2.2H20Na2CO3.H20Na2CO3.10H20Na2CO3. Na2CO3.10H20Na2CO3.10H20Na2CO3.10H20Na2CO3.	WATER NANPO2CC3(s) Na+ Cl- CC3= HCC3- OH- NpO2(CC3)2=- NPO2(CC3)3=- CC2(aq) NPO2CC3- NPO2CC3- NPO2CH(aq) H+ NPO2(0H)2- Trona Thermonatrite 2CC3-Reptahydrate Natron Natron	Molality 8.32153E-01 9.87386E+00 5.56057E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10 1.28920E-10 9.80463E-12 4.35852E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	7.78985E-01 1.0000E+00 5.2769JE+00 5.21732E+00 6.1380IE-04 5.04583E-04 2.08552E-04 3.3404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.6012IE-09 1.28920E-10 3.76405E-11 1.29676E-12 1.00000E+00 1.00000E+00 1.00000E+00	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.812 1.955 1.000 3.839 0.2975 1.000 1.000 1.000 1.000	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 4.82083E-04 1.34534E-04 5.21729E-06 2.38320E+05 6.42544E+09 4.73516E+08 2.88282E+10 4.53797E+11 3.45122E+12 1.53420E+12 0.00000E+00 0.00000E+00 0.00000E+00	4.96989±01 8.84042±00 5.02295±00 4.97858±00 2.12246E-02 1.22622±-03 3.42198E-04 1.32706±-05 1.63436±-08 1.20442±-07 7.33267±-10 8.77844±-12 3.90234±-12 0.000000±00 0.00000±+00 0.00000±+00
	Species Name H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2+ NpO2OH(aq) H+ NpO2(OH)2- Na2CO3.H20Na Na2CO3.10H20Na CO3CO3- NaC1	WATER NaNp02CC03(s) Na+ Cl- CC3= HC03- OH- Np02(CC3)2=- CC2(aq) Np02CC3- Np02CC3- Np02C(aq) H+ Np02(0H)2- Trona Thermonatrite 2CC3-Heptahydrate Nahcolite	Molality 8.32153E-01 9.87386E+00 5.61012E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10 1.28920E-10 9.80463E-12 4.35852E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	7.78985E-01 1.0000E+00 5.27693E+00 6.13801E-04 5.04583E-04 2.06552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.28920E-10 3.76405E-11 1.29676E-12 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.000 3.839 0.2975 1.000 1.000 1.000 1.000 1.000	1.95390E+01 3.47559E+00 1.97476E+00 1.95732E+00 8.3440E-03 4.82083E-04 1.34534E-04 1.34534E-04 2.38320E-05 6.42544E-09 4.73516E-08 2.88282E-10 4.73516E-08 2.88282E-10 4.53797E-11 3.45122E-12 1.53420E-12 0.00000E+00 0.00000E+00 0.00000E+00	4.96989±01 8.84042±00 5.02295±00 4.97858±00 1.22622=03 3.42198=04 1.32706±05 6.06184±-05 1.63436±08 1.20442±07 7.33267±10 1.154272=10 8.77844±-12 3.90234±-12 0.00000±00 0.00000±00 0.00000±00 0.00000±00
444552344567599012264444842990125	Species Name H20 NahpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CH(aq) H+ NpO2(OH)2- Na2H(CO3)2.2H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20Na2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20NA2HCO3.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.10H20.	WATER NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)3=- NpO2(CO3)3=- NpO2(CO3)3=- CO2(aq) NpO2CO3- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron Natron NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON NATRON	Molality 8.32153E-01 9.87386E+00 5.56057E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10 1.28920E-10 9.80463E-12 4.35852E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 2.08552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.28920E-10 3.76405E-11 1.2967E-11 1.2967E-12 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.812 1.955 1.000 3.839 0.2975 1.000 1.000 1.000 1.000	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 4.82083E-04 1.34534E-04 5.21729E-06 2.38320E+05 6.42544E+09 4.73516E+08 2.88282E+10 4.53797E+11 3.45122E+12 1.53420E+12 0.00000E+00 0.00000E+00 0.00000E+00	4.96989±01 8.84042±00 5.02295±00 4.97858±00 2.12246E-02 1.22622±-03 3.42198E-04 1.32706±-05 1.63436±-08 1.20442±-07 7.33267±-10 8.77844±-12 3.90234±-12 0.000000±00 0.00000±+00 0.00000±+00
444552840078999223400092900 9907285284007899092234000999012550250 99072444865878990922349009899012550250 990825007899012234900988901125555	Species Name H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=x- CO2(aq) NpO2CO3- NpO2+ NpO2OH(aq) H+ NpO2(OH)2- Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.1	WATER NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO4 NpO2CO4(aq) H+ NpO2(OH)2- Trona Thermonatrite 2CO3-Heptahydrate Natron Nahcolite Halite DISABLED DISABLED	Molality 8.32153E-01 9.87366E+00 5.56057E+00 2.37058E-02 1.36556E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.1896E-10 9.80463E-12 4.3552E-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	7.78985E-01 1.00000E+00 5.27693E+00 5.21732E+00 6.13801E-04 2.08552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.28920E-10 3.76405E-11 1.2967E-11 1.2967E-12 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.000 3.839 0.2975 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.95390E+01 3.47559E+00 1.97476E+00 8.34440E-03 4.82083E-04 1.34534E-04 5.21729E-06 2.38320E-05 6.42544E-09 4.73516E-08 2.88282E-10 4.53797E-11 3.45122E-12 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96983E+01 8.84042E+00 5.02295E+00 4.97858E+00 1.22622E-03 3.42198E-04 1.32706E-05 6.06184E-05 1.63436E-08 1.20442E-07 7.33267E-10 1.15427E-10 8.77844E-12 3.90234E-12 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
	Species Name H20 NahpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CH(aq) H+ NpO2(H(2- Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20Na NaCO3.10H20NA NaCO3.10H20NA NaCO3.10H20NA NaCO3.10H20NA NaCO3.10H20NA 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44451344667399012334990012513950	Species Name H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=x- CO2(aq) NpO2CO3- NpO2+ NpO2OH(aq) H+ NpO2(OH)2- Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20Na2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 Na2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.10H20NA2 NA2CO3.1	WATER NaNpO2CO3(s) Na+ Cl- CO3= MpO2(CO3)2=- NpO2(CO3)3=- NpO2(CO3)3=- CO2(aq) NpO2CO3)3=- CO2(aq) NpO2CO3(aq) He NpO2CO4(aq) He NpO2(OH)2- Trona Natron Natron Natrot Natrot Natrot Litrate.base.only NO2CH(amor)	Molality 8.32153E-01 9.87386E+00 5.56057E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10 1.28920E-10 9.80463E-12 4.35852E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0	7.78985E-01 1.00000E+00 5.27693E+00 6.13801E-04 5.04583E-04 2.08552E-04 3.93404E-10 5.78442E-14 5.30275E-08 2.43696E-07 1.60121E-09 1.28920E-10 3.76405E-11 1.29676E-12 1.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9361 1.000 0.9406 0.9383 2.5892E-02 0.3684 0.5457 2.6542E-05 8.5436E-10 2.905 1.812 1.955 1.000 3.839 0.2975 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.95390E+01 3.47559E+00 1.97476E+00 1.95732E+00 8.3440E-03 4.82083E-04 1.34534E-04 1.34534E-04 2.38320E-05 6.42544E-09 4.73516E-08 2.88282E-10 4.73516E-08 2.88282E-10 4.53797E-11 3.45122E-12 1.53420E-12 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96989±01 8.84042±00 5.02295±00 4.97858±00 1.22622=03 3.42198=04 1.32706±05 1.63436±08 1.20442±07 7.33267±10 1.154272=10 8.77844±12 3.90234±-12 0.00000±00 0.00000±00 0.00000±00 0.00000±00 0.00000±00 0.00000±00 0.00000±00
4 444 44 44 44 44 44 44 44 44 44 44 44	Species Name H20 NahpO2CO3(s) Na+ C1- C03= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2(DH)2- Na3H(CO3)2.2H20_ 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NaNpO2CO3(s) NCO3= CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CH(a) H+ NpO2(H)2- Trona Thermonatrite Natron Natron Natron Litrate.base.only NpO2OH(amor) NpO2OH(amor)	Molality 8.32153E-01 9.87386E+00 5.61012E+00 2.37058E-02 1.36956E-03 3.82200E-04 1.48219E-05 6.77047E-05 1.82542E-08 1.34522E-07 8.18986E-10 1.28920E-10 9.80463E-12 4.35852E-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 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 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4 444 444 444 444 444 444 444 444 444	Species Name H20 NahpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CH(aq) H+ NpO2(H)2- Na2H(CO3)2.2H20_Na Na2CO3.10H20_Na Na2CO3.10H20_Na Na2CO3.10H20_Na Na2CO3.10H20_Na Na(CO3)2.2H20_Na Na2CO3.10H20_Na Na2CO3.10H20_Na Na2CO3.10H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na Na(CO3)2.2H20_Na 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	Species Name H20 NahpO2CO3(s) Na+ C1- C03= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CH(aq) H+ NpO2(OH)2- Na2CO3.10H20Na Na2CO3.10H20Na NaCC1NaCO3_10H20Na NaCH(aq)to.1 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<pre>4 44444444444444444444444444444444444</pre>	Species Name H20 NahpO2CO3(s) Na+ C1- C03= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CH(aq) H+ NpO2(OH)2- Na3H(CO3)2.2H2ONai Na2CO3.10H2ONai Na2CO3.10H2ONai Na2CO3.10H2ONai Na2CO3.10H2ONai Na2CO3.10H2ONai Na2CO3.10H2ONai Na2CO3.10H2ONai Na2CO3.10H2ONai Na2CO3.10H2ONai Na0H(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) HC1(aq)to.1 NpO2CH(aged) 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901138490789091204414444445555555555555555555555555555	Species Name H20 NahpO2CO3(s) Na+ C1- C03= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3- NpO2(OH)2- Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na NaCC3Na NaCC3Na NaCC3Na NaCC3Na NaCC3Na NaCC3Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NaCH(agc)Na NoTES: - Water 'r - Gas 'mO - Descrig 'dG/RT/'_ * Saturai	WATER NaNpO2CO3(s) NaNpO2CO3(s) CO3 HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CH(aq) H+ NpO2(H)2- Trona Thermonatrite 2CO3-Reptahydrate Natron Natron Natron DISABLED_DISABLED Litrate.base.only NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) 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901138490789091204414444445555555555555555555555555555	Species Name H20 NaMpO2CO3(s) Na+ C1- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2(All 2- Na3H(CO3)2.2H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na NoTES - Nater '' - 'Descrif * Saturat * Saturat * Saturat * Saturat * Saturat	WATER NaNpO2CO3(s) NaNpO2CO3(s) CO3 HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CH(aq) H+ NpO2(H)2- Trona Thermonatrite 2CO3-Reptahydrate Natron Natron Natron DISABLED_DISABLED Litrate.base.only NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) NpO2CH(amor) 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# Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT

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í	6 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Total G/ Flashing # invers	6236092E+03 # 14 Ech pblm	22			
	\$\$000	LBenchmark TITRO DATABASE: HEWR 95.01.31 Am(1 Pressures	Problem, LOG10 o W86; Np(V)-Na-CO -Na-Cl-CO3-SO4-F -Na-Cl-CO3-SO4-F 1.0000000000 [=]	DELION: NP(V)OZ WIEH C) 03-0H-C1-C1O4 (NR94); 04 (FRSR89,FRF90,F91); ATM Temperature=	03 11 5.61mo Refr92,Rff94 2.98E+02	NaCl FF94) ] Xelvin	- CA 144
		Elemental Abun	dances for Flash Probl	olem			
		Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter		
		3.92881252£+01 3.70599297±+01		9.94024309£+01 4.97975186E+01			
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	5.5		a in	0.00000000E+00 4.95987023E+00		Chlorine	
			0 10	0.0000000E+00 3.21548707E-02			
			00	0.00000000E+00 0.00000000E+00	~ ~	Poslon Necton	
			00	0.0000000000000000000000000000000000000			
	181		00	00+30000000 0	0.0000000E+		
	52			0,00000000E+00 D.0000000E+00		TracerEl Th(IV)	
			00	0.00000000E+00 0.00000000E+00	00		
	n i		нс	1.39091324E-04 0.00000000E+00	3.29713479E+	Np (V) C104= (EL)	
			0.0000000000000000000000000000000000000	0.00000000E+00	0.00000000E+0		
		-8,00005678E-1	6 ~2.260635	-2.024085115-15	• •	Charge	
		Solution	cers, Calculated				
		H20 MAS TDS(g/k	327,57686846059	.97 grams .97 grams .94 g/kgH20			
(		Specified Solu DENSITY	tion Density 1188.66091947	607 kg/m^3 #	g/1		
		S	eters 0	ed De			
	5.0		יע	6			
		Density based Percent relat	on TDS and NaCl so we error vs NaCl d	lutions 1188.66 ensity 0.00000	1188.66091947607 g .00000000000000E+000 %	7/ .	
		TARLE OF	сомпрытиясь вов выти с	Action Sector			
				Molality	activity a	But Chef	Total
	ŝ			•			
	a)	HZO NaNp02C03 (s)	WATER NaNpO2CO3 ( s )		.79391E-00	1.9365 1.000 	1.964
		ខ្មែរ	211-		.18493E+00		1-960
	52	CO3= HCO3-	- CO3+	3.39812E-02 1.48672E-03	.78458E-04 .46468E-04	2.5851E-02 ).3676	56.20
		0H- Np02 (CO3 ) 2=-	0H- Np02 (CO3) 2=-	5.046198-04 2.100288-05	ខ្មែន	0.5464 2.683lE-05 0.62501 10	
		CO2 (aq)	CO2 (aq)	1.49488E-08	.34356E-08	2.906	5.290
			Npo2+	5.77122E-10	11979E-09	1.940	2 0 2
				7.48733E-12 7.48733E-12	.194036E-11 .84836E-11	3.804	2.6496
	ŝ	Na3H(CO3)2.2H20	zz (HO) ≥ Doga	0.000002+00	.0000000+000	1.000	0000 O
		Na 2C03 . H20 Na 2C03 . 7H20	Thermonatrite Na2C03-Heptahydrate	0,00000E+00	.000000E+00	1.000	0000.0
		Na 2CO3 . 10H20 NaHCO3	Sa rel	0.00000E+00 0.00000E+00	.00000E+00	1.000 1.000	0.000
		NaCI Na 3Np02 (CO3) 2	Halite (s)_DISABLED_DISABLED		.000000E+00	1.000	0.000
		NpO20H ( amor )	Np020H (amor)		000000000000000000000000000000000000000	1.000	0.000
	t Ali E Si f	Np020H(aged) HCl(aq)to	.to.titrate.acid.only	00	.00000E+00	1.000	0.000
	è.						



Species Name	Molality	Activity	Act Coef	Total Moles	Molarîty	mg/liter	Descriptor
H20 WATER	8.32282E-01	7.79391E-01	0.9365	1.96437E+01	4.97003E+01	8.95361E+05	
2 NaNp02C03 (s)	9.82115E+00	1.000000+00	1.000	3.47556E+00	8.79348E+00	3.09571E+06	
Na+ Na+	5.61021E+00	5.27230E+00	0.9398	1.98537E+00	5.02316E+00	1.15481E+05	
21- CI-	5.53952E+00	5.18493E+00	0.9360	1.96035E+00	4.95987E+00	1 75842E+05	
CO3= CO3=	3.39812E-02	8.78458E-04	2.5851E-02	1.20255E-02	3.04255E-02	1.82581E+03	
C HCO3+ HCO3-	1.48672E-03	5.46468E-04	0.3676	5.26128E-D4	1.33115E-03	8 12230E+01	
CH- OH-	5.04619E-04	2.75741E-04	0.5464	1.78577E-04	4.51816E-04	7 68417E+00	-1.22E-09
V 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
Npo2 (C03) 3==- Npo2 (C03) 3==-	1.34208E-04	1.18584E-13	8.8359E-10	4.74943E-D5	1.20165E-04	5 39629E+01	2.62E-09
<ul> <li>CO2 (aq)</li> <li>CO2 (aq)</li> </ul>	1.49488E-08	4.34356E-08	2.906	5.29018E-09	1.33846E-08	5 89054E-04	-7.17E-08
Npo2co3- Npo2co3- Npo2co3-	1.34916E-07	2.43910E-07	1.808	4.77447E-08	1.20798E-07	3 97494E-02	5.29E-12
2 Np02+ Np02+	5.77122E-10	1.11979E-09	1.940	2.04235E-10	5.16733E-10	1 39025E-04	-1.25E-09
% Np020H (aq) Np020H (aq)	1.192058-10	1.19205E-10	1.000	4.21850E-11	1.067328-10	3 05311E-05	3.27E-08
	7.48733E-12	2.84836E-11	3.804	2.64966E-12	6.70386E-12	6 75682E-09	-3.39E-08
% 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
Trona Trona (CO3) 2.2H20	0.000002+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0 000002+00	-3.32E+00
🕇 Na2CO3.H20 Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	D 00000E+00	-2.20E+D0
% Na2CO3.7H20 Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.000005+00	0.00000E+00	0 00000E+00	-1.91E+00
10H20	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0 000001000	-1.87E+00
NaHCO3 NaHCO3	0.00000E+00	1.000002+00	1.000	0.00000E+00	0.000005+00	0 00000E+00	-2.14E+00
NaCl Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0 00000E+00	-1.34E-01
Na3Np02 (C03) 2 (s) _DISABLED_DISABLED	0.000005+00	1.00000E+00	1.000	D. DOCOOE+00	0.000000+00	0 00000E+00	-9.302+02
to titre	0.00000E+00	0.00000E+00	1.000	0.000005+00	0.00000E+00	0 00000E+00	-2.93±+02
<pre>// NpO20H(amor)NpO20H(amor)</pre>	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0 00000E+00	-3.792+00
% Np020H (aged) Np020H (aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0 00000E+00	-3.20E+00
F HCl (aq)to.titrate.acid.only F	0.00000E+00	0.000005+00	1.000	0.0000000+00	0.00000E+00	0 00000E+00	-2.506+02
	11 1764						

pH = -log[a(H+)] =
Osmotic Coefficient*
Equilibrium RH (%) =
Ionic Strength (m) = u 288552 288552

10.5454 1.236838 77.939147 5.645593

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		(1) N O D			·		
Appendix N: S	ample Output File	"Np_NaCI_B	M_LOG.OU	Γ'			
3 Density, kg/m3	= 1188.66						
	<pre>*molality* is mole :</pre>	fraction H2O in	aqueous phase				
- Gas "p	blality and activ						
	iptor* means: /lnl0 for species w	ith mongero con	/		•		
	ation Index for min			ce criterion;			
	(activity) for aque			oncentrations			
*log10	(partial pressure) :	for gases					
Total G/RT= -	4.67449693E+03						
Flashing Titrati							
# inversions for	batch pblm	22					
	E Problem, LOG10 op:			imolal NaCl	FMT V2.0		
	/FW86; Np(V)-Na-CO3- I)-Na-Cl-CO3-SO4-PO4	4 (FRSR89, FRF90,	991.RFFR92.RF	P94.RRFF94)			
Pressure=	1.00000E+00 [=] A1	M Temperatu		02 [=] Kelvir	1		
; Slemontal Numda	nces for Flash Probl						
STEREICAL NOUNDA	nces for riash riob.	(Cal					
Total Moles	Ag Molality	Aq. Molarity	Aq. mg/lites	-			
3.95867206E+01 3.72253652E+01		9.94062599E+01	1.00191569E				
5.47601956E+00		4.98398335E+01 5.02347422E+00	7.97407433E- 1.15488517E-				
0.0000000E+00		0.00000000E+00	0.00000000		ı		
0.0000000E+00		0.0000000E+00	0.0000000E+	00 Magnesium			
0.00000000E+00 1.96468480E+00		0.00000000E+00	0.0000000E+				
0.00000000E+00		4.93352227E+00 0.00000000E+00	1.74908165E4 0.00000000E4				
3.49364905E+00		4.55413352E-02	5.46996977E4				
0.0000000E+00		0.0000000E+00	0.0000000E+				
0.00000000E+00 0.00000000E+00		0.0000000E+00	0.0000000E+				
0.00000000E+00		0.00000000E+00 0.0000000E+00	0.00000000E+ 0.00000000E+				
0.0000000E+00		0.0000000E+00	0.00000000E+				
0.0000000E+00		0.0000000E+00	0.000000000				
0.0000000E+00 0.0000000E+00		0.0000000E+00	0.00000000E+				
0.00000000E+00		0.00000000E+00 0.0000000E+00	0.0000000E+ 0.00000000E+				
3.47561578E+00		2.57965074E-04	6.11501564E+				
0.0000000£+00		0.0000000E+00	0.0000000E+				
0.0000000E+00 0.0000000E+00		0.0000000E+00	0.0000000E+		s		
		0.00000000E+00 4.67868728E-15	0.00000000E+ 0.00000000E+				
				·· ·····			
	ters, Calculated	_					And the state of the second
SOLUTION MASS H20 MASS	473.33968453363 356.57400341759						1 23
TDS(g/kg)	327.46549102542						Y
						9	
Specified Solut		F 1 ( 4-7	- (7				
DENSITY	1188.6038311184	5 kg/m^3 =	g/1				
Solution Parame	ters Based on Speci:	fied Density					N. C. S.
SOLUTION VOL	0.39823166654968	1 liters					· · · · · · · · · · · · · · · · · · ·
TDS	293.21043735098	4 g/l					
Density based o	n TDS and NaCl solut	tions 1188.60	383111845	g/l			
	e error vs MaCl den:		00000000000E+00				
TABLE OF CONCENTR	ATIONS FOR BATCH SYS	STEM .					
		(					
Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter
H20			7 700/0				
H20 NaNp02C03(s)	WATER NaNpO2CO3(s)	8.32465E-01 9.74696E+00	7.79962E-01 1.00000E+00	0.9369 1.000	1.97930E+01	4.97021E+01	8.95393E+05
Na+	Na+	5.61035E+00	5.26665E+00	0.9387	3.47551E+00 2.00051E+00	8.72736E+00 5.02347E+00	3.07243E+06 1.15489E+05
C1-	C1-	5.50989E+00	5.138842+00	0.9327	1.96468E+00	4.93352E+00	1.74908E+05
CO3= HCO3-	C03≂	4.83971E-02	1.24807E-03	2.5788E-02	1.72571E-02	4.33344E-02	2.60046E+03
HCO3- OH-	HC03- OH-	1.63010£-03 6.55397E-04	5.97114E-04 3.58792E-04	0.3663 0.5474	5.81251E-04	1.45958E-03	8.90593E+01
Np02 (C03) 2=-	Np02 (C03) 2=-	2.94209E-05	3.58792E-04 8.01487E-10	0.5474 2.7242E-05	2.33698E-04 1.04907E-05	5.86839E-04 2.63433E-05	9.98054E+00
Np02(C03)3==-	Np02(C03)3==-	2.58546E-04	2.39623E-13	9.2681E-10	9.21906E-05	2.31500E-04	1.02493E+01 1.03961E+02
Np02003-	Np02C03-	1.35468E-07	2.44172E-07	1.802	4.83043E-08	1.21297£-07	3.99135E-02
CO2 (ag) NpO2+	C02 (ag)	1.25492E-08	3.64751E-08	2,907	4.47472E-09	1.123652-08	4.94515E-04
NpO20H(ag)	NpO2+ NpO2OH(aq)	4.11022E-10 1.09291E-10	7.89015E-10 1.09291E-10	1.920 1.000	1.46560E-10 3.89705E-11	3.68027E-10 9 78589E-11	9.90165E-05
H+	H+	5.83272£-12	2.19064E-11	3.756	2.07980E-12	9.78589E-11 5.22258E-12	2.79929E-05 5.26384E-09
Np02 (OH) 2-	NpO2 (OH) 2-	6.38945E-12	1.89128E-12	0.2960	2.27831E-12	5.72107E-12	1.73384E-06
Na3H(CO3)2.2H2O Na2CO3.H2O	Trona Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00
	2C03-Heptahydrate	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00
Na2CO3.10H20	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00 0.00000E+00
NahCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00

1.000 1.000 1.000 1.000 1.000

0.00000E+00 0.00000E+00

0.00000E+00 0.00000E+00

0.00000E+00 0.00000E+00

0.00000E+00

0.00000E+00

1.00000E+00 1.00000E+00 0.00000E+00

 555
 Nalcol.10n20

 556
 Nahcolite

 700
 Nacl

 701
 Nacl

 702
 Nacl

 703
 Nacl

 704
 Nacl

 705
 Nacl

 706
 Nacl

 707
 Nacl

 708
 Nacl

 709
 Nacl

 700
 Nacl

 700
 Nacl

 701
 Nacl

 702
 Nacl

 703
 Nacl

 704
 Nacl

0.00000E+00

0.00000E+00

0.00000E+00

Descriptor

-1.54£-09 9.68E-10

2.18E-09 6.09E-12 -8.67E-08

-1.07E-09

3.69E-08 -3.80E-08 7.50E-08

-3.13E+00

-1.76E+00 -1.72E+00 -2.10E+00

-1.38E+01 -9.30£+02

-2.93E+02

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

Appendix N: Sample Output File "Np_NaCl_BM_LOG.OUT"

- ....

1723	NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.83E+00
7.1	Np020H (aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.0000E+00	0.00000£+00	-3.23E+00
711	HC1(aq)to	.titrate.acid.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.0000E+00	0.00000E+00	-2.50E+02
71 E.									
177	pmH = -log(m/H+)	3 .	= 11.2341						
27.5	$pH = -log\{a(H+)\}$	± 10,6594							
(70)	Osmotic Coeffic:	ent= 1.234823		1					
1213	Equilibrium RH	8) = 77.996177				•			
12.1	Ionic Strength	m) ≈ 5.661425							
17.2	Density, kg/m3	≈ 1188.60							
1717									
	NOTES: - Water	"molality" is mole	fraction H2O in a	queous phase					
1211	- Gas *1	olality and acti	vity are gas part	ial pressures					
1213	- Desci	iptor means:							
		/ln10 for species	with nonzero concs	. (convergence	criterion)				
· * * 2	*Satu	ation Index for mi	nerals, SI#log10(I	LAP/Ksp)					
2:0	*log1	(activity) for acu	eous species with	very small con	centrations				
2.155	*log1(	(partial pressure)	for gases						
17.1									
		4.69179003E+03							
143		me is U1:[SCBABB.F							
12.4	MOLES file na	me is Ul:[SCBABB.F	MT.USERGUIDE]NP_NA	CL_BM_LOG.MOLE	5;1				



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Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

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See Table 27 for explanation of this listing.
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7,			MT.USERGUIDE)NP_N		20.1					
	INGUESS file name OUTFUT file name									
	CHEMDAT file name				1					
	Temperature is Har									
	Benchmark TITRATE			ith CO3 in 5.61mc	lal NaCl FM	nr v2.0				
	DATABASE: HMW84/F									
	95.01.31 Am(III)				RRFF94)					
~										
٠,										
::			•••••	• • • • • • • • • • • • • • • • • • • •	**********	********	*********	*********	*********	*******
~ <u>~</u>	*** ECHO PRINT OF									
			***							
*	•••••		•••••							*******
۰ <i>۴</i>										
- 2	TITRATION Problem:									
	-) Assigning all		7							
20	-) Setting NONREA	CTIVE Porcsity to	0.0							
23										
сņ										
23										
	Specifying VARIABL	E POROSITY FOR T.	ITRATION Problem							
27 28										
	Aqueous Density is	a Emerion of Co	omoosition							
28	when the second is									
	RHOMIN file name	is U1: (SCEABE.F	MT. USERGUIDE   FMT	HWW_NP_AM.RHOMIN;	1					
· ·										
2 E	******	******	**************	• • • • • • • • • • • • • • • • • • • •	**********	*********	*********	********	*********	*******
22	*** TABLE OF MINER									
22	***	SEE APPENDIX L		***						
04 7.6	******						*********	*********	*********	*******
36	GRID BLOCK VOLUMES	in liters								
	1.00E+00 1.00E+0		05+00 1 005+00 -	1 006+00 1 00E+0	0 1 00E+00	2 00E+00	1.005+00	1 008+00	1 005+00	1 005+00
	1.00E+00 1.00E+0							11000.00	1.002.00	1.002.00
23		-								
45	1.00E+00 1.00E+0	0 1.00E+00 1.00	0E+00 1.00E+00 3	1.00E+00 1.00E+0	0 1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
2 ÷ -	1.00E+00 1.00E+0	0								
42										
	1.00E+00 1.00E+0		DE+00 1.00E+00 :	1.00E+00 1.00E+0	0 1.00E+00	1.00E+00	1.00£+00	1.00E+00	1.00E+00	1.00E+00
	1.002+00 1.002+0	0								
45	<pre># inversions for b</pre>	arch mhlm	50							
	Benchmark TITRATE			th CO3 in 5.61mo	lal NaCl FM	T V2.0				
	DATABASE: HNW84/F									
	95.01.31 Am(III)				RRFF94)					
50	Pressure*	1.00000E+00 [#] J	ATM Temperatur	e= 2.98E+02	[=] Kelvin					
ö1										
52	Elemental Abundance	es for Flash Prob	olem							
55 53	Total Meles	No. Molalisa	Aq. Molarity	An mallitar						
	Total Moles	ny. NULALLLY	my. mondarity	Aq. mg/liter						and the second
28	1.11017363E+02	1.11029658E+02	1.00100314E+02	1.008911076+05	Hydrogen				r .	State Chan
57	6.15086815E+01								×.	
53	5.61000000E+00									
59 59	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	Potassium				5	
8 C+	0.0000000E+00								-	
£ 1	0.0000000E+00								·	
	1.61000000E+00								•	~ /
6.3	0.0000000E+00	0.0000000000000000000000000000000000000	0.0000000E+00	0.0000000E+00	Sulfur				٩,	and the second sec
	2.00000001E+00	2.00022150E+00	1.80332719E+00	2.16597629E+04	Carbon					'n
6.E 6	0.00000000000000	0.00000002+00 0.00000002+00	0.0000000E+00 0.0000000E+00	0.0000000E+00 0.0000000E+00	Posion					
€C. €`	0.00000000E+00 0.0000000E+00	0.00000000E+00	0.00000000E+00	0.0000000E+00	Neglon Air					
i titi	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					
?>	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	TracerEl					
7.	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000£+00	Th(IV)					
÷ź.	0.00000002+00	0.0000000E+00	0.00000000000000	0.00000000E+00	Am(III)					
93	0.0000000E+00	0.0000000E+00	0.00000000000+00	0.0000000E+00	U(VI)					
74	0.0000000E+00	0.0000000E+00	0.000000000000000	0.0000000000000000000000000000000000000	Np(V)					
75 75	0.0000000E+00	0.0000000E+00	0.00000000E+00	0.0000000E+00	C104-(EL)					
? > 7 ?	0.0000000E+00	0.00000000E+00	0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00	Phosphorus Electron					
78 78	0.0000000E+00 -2.22044605E-15	0.00000000E+00 -2.22069196E-15	-2.00209536E-15	0.00000000E+00	Charge					
20					2002 90					
2	Solution Paramete	ers, Calculated								
51	SOLUTION MASS	1306.070339098	90 grams							
2	H20 MASS	999.8892657174	86 grams							

#### Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

8.3 306.214981877726 a/kaH20 TDS(q/kq)84 95 23 Specified Solution Density 1177.63607439302  $k\alpha/m^3 = \alpha/1$ DENSITY έć Solution Parameters Based on Specified Density SOLUTION VOL 1.10906108219550 2.5 liters ς, 276.072326670473 g/1 TDS 1177.63607439302 < 2 Density based on TDS and NaCl solutions a/1 Percent relative error vs NaCl density C.00000000000000E+000 % 1.2 С 3 У 4 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM 0 Se Species Name Molality Activity Act Coef Total Moles Molarity mg/liter Descriptor WATER 8.57464E-01 8.59843E-01 H20 1.003 5.55025E+01 5.00446E+01 9.01564E+05 5.61062E+00 3.69881E+00 N&+ 0.6593 5.61000E+00 5.05833E+00 1.16290E+05 Na+ 1.79778E+00 103 CO3= 104 Cl-CO3= 1.99407E+00 4.09214E-02 2.0522E-02 1.99385E+00 1.07884£+05 1.61018E+00 1.06477E+00 C1-0.6613 1.61000E+00 1.45168E+00 5.14664E+04 0.2587 нсознсоз-6.14734E-03 1.59044E-03 6.14666E-03 5.54222E-03 3.38170E+02 6.14665E-03 2.36850E-09 OH-6.14733E-03 4 86901E-03 0.7921 5.54221E-03 9.42580E+01 OH-2.00E-11 . .. CO2 (ag) 2.36876E-09 7.15913E-09 CO2 (aq) 3.022 2.13559E-09 9.39868E-05 ~2.12E-07 1.77959E-12 -8.58E-08 H+ 2.39954E-12 0.7416 2.39927E-12 2.16334E-12 2.18043E-09 H+ 1. Na3H(C03)2.2H20_ 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 0.00000£+00 0.00000E+00 0.00000E+00 11 ~2.52E+02 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 NaOH(ag)....to.titrate.base.only 0.00000E+00 -2.92E+02 ____Nahcolite - - 3 1.00000E+00 NaC1 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.0000E+00 ~9.75E-01 1.00000E+00 NaHCO3 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 ~1.83E+00 Na2CO3.7H20___Na2CO3-Heptahydrate 0.000002+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000£+00 -2.51E-01 Thermonatrite 110 1.00000E+00 0.00000E+00 Na2CO3_H2O 0.00000E+00 1.000 0.00000E+00 0.00000E+00 -7 99E-01 Na2CO3,10H20____ Natron 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 ~8.30E-02 11.6199 11.7497 Osmotic Coefficient= 0.908418 Equilibrium RH (%) = 85.984284 Ionic Strength (m) = 7.604695 52 1177.64 '22 Density, kg/m3 325 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) 129 130 *Saturation Index for minerals, SI=log10(IAP/Ksp) *log10(activity) for aqueous species with very small concentrations *log10(partial pressure) for gases 103 Total G/RTB -6.42133776E+03 • • • • Reaction # 1 sldsum 2.00000000000000 : 97 This is a solid-only reaction 
 >>>
 shifting left by
 4.64434654478255

 109
 calling makenuv for allomorphic reactions

 141
 makenuv for blog
 75
 4.64434654478256 # inversions for batch pblm 1Benchmark TITRATE Problem, LINEAR option; Np(V)02 with CO3 in 5.61molal NaC1 FMT V2.0 22 DATABASE: HMW84/FW86; Np(V)-Na-C03-OH-C1-Cl04(NF44); "~> 95.01.31 Am(III)-Na-C1-C03-S04-P04 (FRSR89,FRF90,F91,RFFR92,RFF94,RRFF94) 144 1.00000E+00 [=] ATM 2.98E+02 [=] Kelvin Pressure= Temperature= 137 146 Elemental Abundances for Flash Problem - 15 Total Moles Ag. Molality Aq. Molarity Aq. mg/liter 563 190 1.11017591E+02 9.93838868E+01 1.00169020E+05 Hydrogen 1.11018363E+02 5.55113597E+01 7.95078006E+05 1.05508682E+02 4.96942389£+01 Oxygen 122 1.5610000E+02 5.61057382E+00 5.02263316E+00 1.15469181E+05 Sodium 0.0000000E+00 0.0000000E+00 0.0000000E+00 Potassium :63 0.0000000E+00 7 A.L 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 Magnesium - 55 0.0000000E+00 0.00000000E+00 Q.0000000E+00 Calcium 156 157 5.61096098E+00 5.02297975E+00 1.78079701E+05 Chlorine 5.61100000E+00 0.0000000E+00 6.58946152E+00 Sulfur 0.0000000E+00 0.0000000E+00 0.0000000E+00 123 6.12839261E-04 Carbon 1.00000005+01 5.48618892E-04 15. 16. 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Posion 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000000000000 Negion 0.00000000E+00 Air 0.0000000E+00 0.0000000E+00 0.0000000E+00 - . -0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Boren 101 0.0000000E+00 0.0000000E+00 0.0000000E+00 0 0000000E+00 Bromine •e4 0.0000000E+00 0.0000000E+00 0.00000000E+00 TracerEl 0.0000000E+00 4 - N ( 0.0000000E+00 0.0000000E+00 0.0000000E+00 Th(IV) 0.0000000E+00 - 1. 0.000000002+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Am(III) 2.17 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 U(VI) 1.00000000E+01 6.12839261E-04 0.00000000E+00 5.48618892E-04 1.30049121E+02 Np(V) ٠*;*; 0.0000000E+00 C104-(EL) 0.0000000E+00 0.0000000E+00 173 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Phosphorus 0.00000000E+00 0.00000000000000 0.00000000E+00 0.00000000E+00 Electron -2.37316632E-15 -2.37314981E-15 -2.12446380E-15 0.0000000E+00 Charge

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# Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

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	Solution Paramete	rs, Calculated							
. 7.	SOLUTION MASS	1328.11614865142	grams						
176	H20 MASS	1000.00695466819	grams						
127	TDS(g/kg)	328.106912108529	g/kgH2O						
74 179	Specified Solutio	n Density							
	DENSITY	1188.93254605477	kg/m^3 =	g/l '		•			
102		rs Based on Specif							
3.1	SOLUTION VOL	1.11706602116201							
5- *0	TDS	293.724084134187	g/1						
190 190	Density based on	TDS and NaCl solut	ions 1188.93	254605477	g/1				
• 77		error vs NaCl dens		000000000E+000					
1.1.1									
183 195									
	TABLE OF CONCENTRAT	TONS FOR BATCH SYS	TEM						
· •									
· 9's	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
194			0 218225 01	7 77050# 01		6 550010.01	4 050185-01	8 953995.95	
	H20	WATER NaNpO2CO3(s)	8.31822E-01 9.99932E+00	7.77959E-01 1.00000E+00	0.9352	5.55091E+01 9.99939E+00	4.96918E+01 8.95147E+00	8.95208E+05 3.15133E+06	
??? -7	NaNp02C03(s)	Nakpozcos(s) C1-	5.61096E+00	5.29329E+00	0.9434	5.61100E+00	5.02298E+00	1.78080E+05	
1. 1. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2.	Na+	Na+	5.61057E+00	5.29268E+00	0.9433	5.61061E+00	5.02263E+00	1.15469E+05	
199	Np02+	Np02+	6.12705E-04	1.21978E-03	1.991	6.12709E-04	5.48499E-04	1.47572E+02	
200	CO2 (ag)	CO2 (aq)	3.86103E-04	1.12115E-03	2.904	3.86106E-04	3.45643E-04	1.52117E+01	1 360 44
201	HCO3-	HCO3- Np02CO3-	2.26571±-04 1.33526E-07	8.38810E-05 2.42971E-07	0.3702	2.26573E-04 1.33527E-07	2.02829E-04 1.19534E-07	1.23760E+01 3.93334E-02	4.26E-09 -1.99E-11
212	Np02C03- H+	ND02403- H+	1.21872E-06	4.78095E-06	3.923	1.21873E-06	1.09101E-06	1.09962E-03	-4.38E-08
203	C03=	C03=	3.09384E-08	8.03342E-10	2.5966E-02	3.09386E-08	2.76963E-08	1.66203E-03	-1.62E-07
.05	OH-	CH-	3.01685E-09	1.63977E-09	0.5435	3.01687E-09	2.70071E-09	4.59318E-05	2.552-08
	NpO2OH(aq)	NpO20H(aq)	7.72186E-10	7.72186E-10	1.000	7.72191E-10	6.91267E-10	1.97740E-04	1.87E-07
207 202	Np02 (C03) 2=-	Np02 (C03) 2=- Np02 (OH) 2-	1.98384E-11 2.04382E-16	5.13354E-16 6.10703E-17	2.5877E-05 0.2988	1.98385E-11 2.04383E-16	1.77595E-11 1.82964E-16	6.90960E-06 5.54494E-11	-1.62E-07 2.13E-07
200	NpO2 (OH) 2- NpO2 (CO3) 3==-	Np02 (C03) 3==-	1.25197E-16	9.87896E-26	7.8908E-10	1.25198E-16	1.12077E-16	5.03310E-11	-3.23E-07
210	Np020H (aged)	NpO20H(aged)	0.00000E+00	1.00000E+00	1.000	0.00000±+00	0.00000E+00	0.00000E+00	-2.38E+00
2**	NaOH(aq)to.ti		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.99E+02
212	HCl(aq)to.ti		0.00000E+00	0.00000E+00	1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-2.45E+02
213 214	Na3NpO2(CO3)2(s)_DI NaC1	SABLED_DISABLED	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1,000	0.00000E+00	0.00000E+00	0.00000E+00	-9.36E+02 -1.23E-01
2:5	Natco3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+00
215	Na2CO3_10H20	Natron	0.000002+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	~7.91E+00
212	Na2CO3_7H20Na2C		0.000002+00	1.00000E+00	1.000	0.0000000+00	0.0000000+00	0.00000E+00	-7.95E+00
212	Na2CO3_H20	Thermonatrite	0.00000E+00 0.00000E+00	1.00000E+00 · 1.00000E+00	1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-8.24E+00 -1.02E+01
213 220	Na3H(CO3)2.2H2O NpO2OH(amor)	Trona NpO20H(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.98E+00
221	Np02011((milet))								
232	pmH ≈ -log[m(H+)]	=	5.9141						
223	pH = -log[a(H+)]	= S.3205							
22:	Osmotic Coefficient Equilibrium RH (%)								
225	lonic Strength (m)								
2.6		= 1188.93							
225									
225	NOTES: - Water "mo	laiity is mole fr lity and "activit							
221	- Descript		y are gas par.	int produces					
2:32	*dG/RT/ln	10 for species wit			criterion)				
2.55		on Index for miner							
2.54		tivity) for aqueou		very small con	centrations				
200 030	-10g10 (pa	rtial pressure) fo	r gabeb						
	Total G/RT= -1.3	3323084E+04							CELEVAN A
2:(9)	Flashing Titration	* 1						. A. T.	1 A
233	# inversions for be	tch pblm	11						
240	1Benchmark TITRATE F DATABASE: HMW84/FW				UNDIAL NACI /	PMI V2.0			
142		Na-C1-C03-S04-P04			4, RRFF94)				1
242		.00000E+00 [=] ATM			2 [=] Kelvin				. *
ý če,									
	Elemental Abundance	es for Flash Proble	m						
245 247	Total Moles	Aq. Molality A	q. Molarity	Aq. mg/liter					
012									
213		······································	.93838868E+01	1.00169020E+0					
250	3.66707638E+01		.96942389E+01	7.95078006E+0					
251 200	5.42543623E+00 0.0000000£+00		.02263316E+00	1.15469181E+0 0.00000000E+0					
253	0.0000000E+00	• •	.00000000E+00	0.00000000E+0					
264			.0000000E+00	0.0000000£+0	0 Calcium				
231	1.95016801E+00		.02297975E+00	1.78079701E+(					
255	0.0000000E+00		.00000000E+00	0.00000000£+0					
255 255	3.47561578E+00 0.00000000E+00		48618892E-04	6.58946151E+( 0.00000000E+(					
200	0.0000000E+00		.00000000000000	0.0000000E+(					
	0.0000000E+00	0.0000000E+00 0	000000006+00	0.0000000E+(	0 Air				
281 262	0.0000000E+00		.00000000E+00	0.0000000E+0					
407	C.000C0000E+00	0.00000000E+00 0	.00000000E+00	5.000000 <u>E</u> +(					

Descriptor

-6.17E-15

6.17E-15

1.85E-14

0.00E+00

-6.17E-15

0.00E+00

0.00E+00

1.23E-14 -3.53E-10

-2.45E+02

-2.38E+00

-2.98E+00

-2.99E+02

-9.36£+02

-1.23E-01

-2.95E+00

-7.91E+00

-7.95E+00

-8.24E+00

-1.02E+01

1.15469E+05

L.52117E+01

L.23760E+01

1.97740E-04

5.90960E-06

5.54494E-11

5.03310E-11

0.00000E+00

) 00000E+00

1.00000E+00

1.00000E+00

0.000002+00

0,00000E+00

0.00000E+00

```
260
        0.0000000E+00
                              0.0000000E+00
                                                   0.0000000000+00
                                                                          0.00000000E+00 TracerE1
                                                    0.0000000E+00
                                                                           0.00000000E+00
                              0.0000000E+00
                                                                                               Th(IV)
10.00
        0.0000000E+00
.
.
        0.0000000E+00
                                                    0.0000000E+00
                                                                           0.0000000E+00
                              0.0000000E+00
                                                                                               Am(III)
100
107
        0.0000000E+00
                              0.0000000E+00
                                                    0.0000000E+00
                                                                           0.0000000E+00 U(VI)
                              6.12839260E-04
                                                     5.48618892E-04
                                                                           1.30049121E+02 Np(V)
        3 47561578E+00
2.52
                              0.0000000E+00
                                                     0.0000000E+00
                                                                           0.0000000E+00
        0.0000000E+00
                                                                                               C104-(EL)
249
270
271
        0.00000002+00
                              0.0000000E+00
                                                    0.00000000£+00
                                                                           0.0000000E+00 Phosphorus
       0.00000000E+00 Electron
                                                                           0.0000000E+00 Charge
072,
01.6
        Solution Parameters, Calculated
ç.,
          SOLUTION MASS 461.602144251012
                                                             grams
270
271
277
277
273
273
                                347.563995068956
                                                              grams
           H20 MASS
                                                             g/kgH20
           TDS(g/kg)
                                 328.106912108175
        Specified Solution Density
                                1188.93254605459
                                                             kg/m^{3} = g/1
           DENSITY
280
244
        Solution Parameters Based on Specified Density
           SOLUTION VOL 0.388249228926247
200
                                                             liters
203
254
284
                                 293.724084133903
          TDS
                                                             g/1
                                                                1188.93254605459
        Density based on TDS and NaCl solutions
                                                                                             g/1
120
                                                             0.000000000000000E+000 %
        Percent relative error vs NaCl density
260
2:09
200
     TABLE OF CONCENTRATIONS FOR BATCH SYSTEM
202 Species Name
                                                        Molality
                                                                          Activity
                                                                                             Act Coef
                                                                                                             Total Moles Molarity
                                                                                                                                                  ng/liter
243
                                                         8.318222-01
                                                                          7.77959E-01
                                                                                                              1.92928E+01
ani 1120
                                            WATER
                                                                                             0.9352
                                                                                                                                4.96918E+01
                                                                                                                                                  8.95208E+05
                                                                                                                                8.95147E+00
5.02298E+00
                                                                                                                                                   3.15133E+06
1.78080E+05
.995 NaNp02C03 (s)_____
                                 _NaNp02C03(s)
                                                         9.99932E+00
                                                                          1.00000E+00
                                                                                              1.000
                                                                                                              3.47540E+00
                                                                                                              1.95017E+00
000
007
                                                         5.61096E+00
                                                                           5.29329E+00
                                                                                             0.9434
     C1-
                                              Cl-
                                                         5.61057£+00
                                                                           5.29268E+00
                                                                                             0.9433
                                                                                                              1.95003E+00
                                                                                                                                 5.02263E+00
                                              Na+
      Na+
2년은 Np02+
                                           Np02+
                                                         6.12705E-04
                                                                           1.21978E-03
                                                                                              1.991
                                                                                                              2.12954E-04
                                                                                                                                5.48499E-04
                                                                                                                                                   1.47572E+02
                                                         3.86103E-04
                                                                           1.12115E-03
                                                                                                              1.34196E-04
                                                                                              2.904
                                                                                                                                3.45643E-04
2-3 CO2(ag)
                                         CO2 (ag)
                                                                                                              7.87481E-05
200 HC03-
                                           HC03-
                                                         2.26571E-04
                                                                           8.38810£-05
                                                                                             0.3702
                                                                                                                                2.02829E-04
001
201
                                                                           4.78095E-06
                                                                                                              4.235828-07
     N+
                                               H+
                                                         1.21872E+86
                                                                                              3.923
                                                                                                                                1.091018-06
                                                                                                                                                   1.09962E-03
                                       Np02C03-
                                                         1.33526E-07
                                                                           2.42971E-07
                                                                                              1.820
                                                                                                              4.640902-08
                                                                                                                                1.19534E-07
                                                                                                                                                   3.93334E-02
     No02C03-
                                                                           8.03343E-10
                                                         3.09384E-08
                                                                                             2.5966E-02
                                                                                                              1.075312-08
                                                                                                                                2.76963E-08
                                                                                                                                                   1.66203E-03
002
                                            C03=
     CO3=
                                                                                                              1.04855E-09
1924
                                                                                                                                2.70071E-09
     OH-
                                              OH-
                                                         3.01685E-09
                                                                           1.63977E-09
                                                                                             0.5435
                                                                                                                                                   4.59318E-05
. 65
                                    Np020H(ag)
                                                         7.72186E-10
                                                                           7.72186E-10
                                                                                              1.000
                                                                                                              2.68384E-10
                                                                                                                                6.91267E-10
     NpO20H (acr)
                                                         1.98384E-11
                                                                           5.13355E-16
                                                                                             2.5877E-05
                                                                                                              6.89511E-12
                                                                                                                                1.77595E-11
200
     Np02 (CO3) 2=-
                                  Np02 (C03)2=
                                                                                                              7.10356E-17
                                                                                                                                1.82964E-16
202
     NpO2 (OH) 2-
                                    NoO2 (OH) 2-
                                                         2.04381E-16
                                                                           6.10703E-17
                                                                                             0.2988
:02
                                                         1.25197E-16
                                                                           9.87897E-26
                                                                                                                                1.12077E-16
                                 Np02 (C03) 3==-
                                                                                             7.8908E-10
                                                                                                              4.35139E-17
     Np02 (CO3) 3==-
30.
                                                         0.00000E+00
                                                                           0.00000E+00
                                                                                              1,000
                                                                                                              0.00000E+00
                                                                                                                                0.00000E+00
                                                                                                                                                   0.00000E+00
      HCl(aq).....to.titrate.acid.only
                                                                                                              0.00000E+00
Np020H (aged)
                                                         0.00000£+00
                                                                          1.00000E+00
                                                                                              1.000
                                                                                                                                0.00000E+00
                                                                                                                                                   ).00000E+00
                                 NoO2OH (aged)
                                                                                                              0.00000E+00
311
     Np020H(amor) _____Np020H(amor)
Na0H(aq)....to.titrate.base.only
                                                         D. D0000E+00
                                                                                                                                0.00000E+00
                                                                           1.00000E+00
                                                                                              1.000
%2 NaOH(aq)....to.titrate.base.only
%2 NaOH(aq)....to.titrate.base.only
%3 NaONpO2(CO3)2(s)_DISABLED_DISABLED_Halite
                                                        0.00000E+00
                                                                           0.00000E+00
                                                                                              1.000
                                                                                                              0.00000E+00
                                                                                                                                0 0000002+00
                                                                                              1.000
                                                                                                              0.00000E+00
                                                                                                                                0.00000£+00
                                                        0.00000E+00
                                                                           1.00000£+00
3:4 NaCl_
                                                         0.00000E+00
                                                                           1.00000E+00
                                                                                              1.000
                                                                                                              0.00000E+00
                                                                                                                                D.00000E+00
NaHCO3
Na2CO3.
Na2CO3.
                                     Nahcolite
                                                        0.00000E+00
                                                                           1.00000E+00
                                                                                              1,000
                                                                                                              0.000008+00
                                                                                                                                0.00000E+00
     Na2CO3.10H20___
                                                                                                              0.00000E+00
                                                                                                                                0.00000E+00
                                                        0.00000E+00
                                                                           1.00000E+00
                                                                                              1.000
                                         Natron
     Na2CO3.7H20___Na2CO3~Heptahydrate
                                                         0.00000E+00
                                                                           1.00000E+00
                                                                                              1.000
                                                                                                              0.00000E+00
                                                                                                                                0.00000E+00
                             _____Thermonatrite
-5 Na2C03.H20
                                                        0.000005+00
                                                                           1.00000E+00
                                                                                              1.000
                                                                                                              0.00000E+00
                                                                                                                                0.00000E+00
                                                                                                                                                   3 00000E+00
     Na3H (CO3) 2.2H20_
                                                         0.00000E+00
                                                                           1.00000E+00
                                                                                                              0.00000E+00
                                                                                                                                0.00000E+00
                                                                                              1,000
                                                                                                                                                   0.00000E+00
                                          Trona
320
37 :
     mH = -\log[m(H+)]
                                                            5.9141
     323
                                         5.3205
223
(1)4
(1)25
220
     Density, kg/m3
                             z
                                      1188.93
32
28
     NOTES: - Water 'molality' is mole fraction H2O in aqueous phase
                - Gas "molality" and "activity" are gas partial pressures
<u>283</u>
230
                - "Descriptor"
                                   means:
33
                   *dG/RT/lnl0 for species with nonzero concs. (convergence criterion)
                   *Saturation Index for minerals. SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
322
322
                   *log10(partial pressure) for gases
144
2.5
Total G/RT=
                        -4.63379813E+03
320 *** SUMMARY INFORMATION FOR ADDITION OF DV(2)...DV(14) WOULD BE HERE ***
. . .
Flashing Titration #
                                              15
     # inversions for batch pblm
                                                       23

        Still
        Description
        Data
        Physical
        Physical
        PMT V2.0
        <th
345
(145
                            1.00000E+00 [=] ATM
                                                                                  2.98E+02 [=] Kelvin
           Pressure=
                                                            Temperature=
385 Elemental Abundances for Flash Problem
25.5
350
                              Ag. Molality
                                                 Ag. Molarity Ag. mg/liter
        Total Moles
```

Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

mg/liter

8.95289£+05 3.14043E+06

1.15468E+05 1.77638E+05 3.28108E+02

6.10225E+01 1.83887E+00 1.35568E+00

1.91755E+00

1.86923E-03 3.94312E-02 7.52738E-04

2.76166E-08

4.02206E-05 4.52501E-07

0.00000E+00 0.00000E+00

0.00000E+00

0.00000E+00 0.00000E+00

0.00000E+00

0.0000DE+00 0.0000DE+004

0.00000E+00

0.00000E+00

0.00000E+00

Descriptor

-1.39E-10 5.14E-10

1.15E-09

-7.11E-09 3.15E-13

-5.05E-10

-3.76E-09 3.26E-09 7.03E-09

-4.19E+00 -2.94E+00

-2.66E+00

-2.62E+00 -2.26E+00

-1.25E-01

-9.31E+02 -2.94E+02

-3.67E+00

-3.08E+00

-2.49E+02

253							
2.1.1	3.87258579E+01	1.11018601E+02	9.93937371E+01	1.00178948E+05			
357	3.67484080E+01	5.55305592E+01	4.97159013E+01	7.95424591E+05			
360	5.43251790E+00	5.61002101E+00	5.02259034E+00	1.15468197E+05	Sodium		
327	0.0000000E+00	0.00000000E+00	0.0000000E+00	0.0000000E+00			
455	0.00000000E+00	0.0000000E+00	0.000000E+00	0.00000000E+00	Magnesium		
353	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	Calcium		
وتبرى	1.95220036E+00	5.59653330E+00	5.01051495E+00	1.77637786E+05	Chlorine		
201	0.00000000E+00	0.00000000E+00	0.0000000E+00	0.00000000E+00	Sulfur		
202	3.47814044E+00	7.24644343E-03	6.48766141E-03	7,79233012E+01	Carbon		
362	0.0000000000000000000000000000000000000	0.00000000E+00	0.0000000E+00	0.0000000E+00			
·	0.00000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00			
1	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.0000000E+00			
		0,00000000E+00	0.0000000E+00	0.0000000E+00			
	0.0000000E+00	0.00000000E+00	0.0000000E+00	0.0000000E+00			
201	0.0000000E+00	0,0000000E+00	0.00000000E+00	0.0000000E+00			
202	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00			
95.0	0.00000002+00	0.00000000E+00	0.0000000E+00	0.00000000E+00			
37.2 477	0.0000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			
	0.0000000E+00		7.87723651E-06	1.86728474E+00			
2	3.47561578E+00	8.79854005E-06	0.00000000E+00	0.0000000E+00			
. 73	0.0000000E+00	0.0000000E+00	0.00000000E+00	0.00000000E+00			
374	0.0000000E+00	0.0000000E+00	0.00000000E+00	0.00000000E+00			
325	0.0000000E+00	0.0000000000000000000000000000000000000	-2.34399998E-15	0.00000000E+00			
376	-9.13270924E-16	-2.010140032-13	-2.3433333306-13	0.00000000000000			
375		ters, Calculated	30 grans				
379	SOLUTION MASS		-				
330	H20 MASS	348.8231479353	-				
321	TDS(g/kg)	327.8273872537	19 g/kgH20				
362							
	Specified Solut			-13			
شردى	DENSITY	1188.789312087	19 kg/m^3 =	g/1			
28°.			Stad Banalas				
080		ters Based on Spec:					
327	SOLUTION VOL	0.3896207043815					
152	TDS	293.5002681204	85 g/l				
				000000000	~/)		
(m)	Density based o	n TDS and NaCl solu			g/1		
201	Percent relativ	e error vs NaCl de	nsity 0.000000	000000000000000000000000000000000000000	ъ		
002							
305							
· · · ·							
	TABLE OF CONCENTR	ATIONS FOR BATCH S	YSTEM				
2							
				The stand has	has coof	Tetal Males	Molarity
293	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity
295 308	-		-	Ţ.			
29) 332 399	H2O	WATER	8.31932E-01	7.78290E-01	0.9355	1.93627E+01	4.96963E+01
200 300 300 400	H2O NaNpO2CO3 (s)	NaNp02C03(s)	8.31932E-01 9.96382E+00	7.78290E-01 1.00000E+00	0.9355 1.000	1.93627E+01 3.47561E+00	4.96963E+01 8.92050E+00
29) 332 399	H2O NaNpO2CO3 (s)	NaNp02C03(s) Na+	8.31932E-01 9.96382E+00 5.61002E+00	7.78290E-01 1.00000E+00 5.28628E+00	0.9355 1.000 0.9423	1.93627E+01 3.47561E+00 1.95691E+00	4.96963E+01 8.92050E+00 5.02259E+00
です。	H20 NaNp02C03 (5) Na+ C1-	NaNp02C03(s) Na+ Cl-	8.31932E-01 9.96382E+00 5.61002E+00 5.59653E+00	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00	0.9355 1.000 0.9423 0.9420	1.93627E+01 3.47561E+00 1.95691E+00 1.95220E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00
200 300 400 400 400 400 400	H20 NaNp02C03 (s) Na+ C1- C03=	NaNp02C03(s) Na+ Cl- C03=	8.31932E-01 9.96382E+00 5.61002E+00 5.59653E+00 6.10711E-03	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04	0.9355 1.000 0.9423 0.9420 2.5954E-02	1.93627E+01 3.47561E+00 1.95691E+00 1.95220E+00 2.13030E-03	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03
学 (1) (1) (1) (1) (1) (1) (1) (1) (1) (1)	H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3-	NaNp02C03(s) Na+ Cl- C03= HC03-	8.31932E-01 9.96382E+00 5.61002E+00 5.59653E+00 6.10711E-03 1.11706E-03	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698	1.93627E+01 3.47561E+00 1.95691E+00 1.95220E+00 2.13030E-03 3.89655E-04	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.00009E-03
393800 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2014 2014 2014 2014 2014 2014 2014	H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3- OH-	NaNp02C03(s) Na+ C1- C03= HC03- OH-	8.31932E-01 9.96382E+00 5.61002E+00 5.59653E+00 6.10711E-03 1.11706E-03 1.20768E-04	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442	1.93627E+01 3.47561E+00 1.95691E+00 1.95220E+00 2.13030E-03 3.89655E-04 4.21267E-05	4.96963E+01 8.92050E+00 5.01051E+00 5.46763E-03 1.00009E-03 1.08122E-04
393800 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2038 2014 2014 2014 2014 2014 2014 2014 2014	H20 NaNpO2CO3(s) Na+ C1- CO3= HCO3-	NaNp02C03 (s) Na+ C1- C03= HC03- OH- Np02 (C03 ) 2=-	8.31932E-01 9.96382E+00 5.61002E+00 6.1071E-03 1.1706E-03 1.20768E-04 3.89199E-06	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.3698 0.5442 2.6056E-05	1.93627E+01 3.47561E+00 1.95691E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==-	NaNp02C03 (s) Na+ C1- C03= HC03- OH- Np02 (C03) 2=- Np02 (C03) 3==-	8.31932E-01 9.96382E+00 5.61002E+00 5.59653E+00 6.10711E-03 1.11706E-03 1.20768E-04 3.89199E-06 4.76942E-06	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.0141E-10 3.85055E-15	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10	1.93627E+01 3.47561E+00 1.95631E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.66368E-06	4.96963E+01 8.92050E+00 5.02259E+00 5.46763E-03 1.0009E-03 1.08122E-04 3.4846E-06 4.27001E-06
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq)	NaNp02C03 (s) Na+ C1- C03= HC03- OH- Np02 (C03) 2=- Np02 (C03) 3=- C02 (aq)	8.31932E-01 9.96382E+00 5.61002E+00 6.1071E-03 1.11706E-03 1.20768E-04 3.89199E-06 4.76942E-05 4.74407E-08	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904	1.93627E+01 3.47561E+00 1.95691E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.66388E-06	4.96963E+01 8.92050E+00 5.02259E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.27001E-06 4.24731E-08
2002 2011 2012 2012 2012 2012 2012 2012	H20 NaNp02C03(s) Na+ C1- C03= HC03- OH- Np02(C03)2=- Np02(C03)3==- C02(aq) Np02C03-	NaNp02C03 (s) Na+ C1- C03= HC03- OH- Np02 (C03 ) 2=- Np02 (C03 ) 3=- C02 (aq) Np02 (aq) Np02 (C03-	8.31932E-01 9.96382E+00 5.61002E+00 6.1071E-03 1.11706E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.74407E-08 1.33846E-07	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.0141E-10 3.85055E-15 1.37761E-07 2.43265E-07	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 2.6056E-05 8.0734E-10 2.904 1.817	1.93627E+01 3.47561E+00 1.95691E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.66368E-06 1.6548E-08 4.66887E-08	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.6763E-03 1.08022E-04 3.48446E-06 4.24731E-08 1.19831E-07
	H20 NaNpO2CO3(s) Na+ Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO3-	NaNp02C03 (s) Na+ C1- C03= HC03- OH- Np02 (C03) 2=- Np02 (C03) 3==- C02 (aq) Np02 (c03) 3=- C02 (aq) Np02C03 Np02C03	8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 1.33846E-07 3.12502E-09	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.0141E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981	1.93627E+01 3.47561E+00 1.95691E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.6568E-06 1.6568E-06 1.65484E-08 4.6687E-08 1.09008E-09	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.66763E-03 1.0009E-03 1.08122E-04 3.8846E-06 4.27001E-06 4.27001E-06 4.24731E-07 1.19831E-07 2.79779E-09
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2C+ H4	NaNp02C03 (s) Na+ C1- C03= HC03- 0H- Np02 (C03) 2=- Np02 (C03) 3=- C02 (aq) Np02C03- Np02+ H+	8.31932E-01 9.96382E+00 5.61002E+00 5.59653E+00 6.1071E-03 1.11766E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.74407E-08 1.3386E-07 3.12502E-09 3.06048E-11	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18952E-09 1.19335E-10	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.6536E-06 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11	4.96963E+01 8.92050E+00 5.02259E+00 5.46763E-03 1.0802E-03 1.08122E-04 3.48446E-06 4.27001E-06 4.2701E-08 1.19831E-07 2.79779E-09 2.74002E-11
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2+ H+ NpO2OH(aq)	NaNp02C03 (s) Na+ C1- C03= HC03- OH- Np02 (C03 ) 2=- Np02 (C03 ) 3==- C02 (c03 ) 3==- C02 (c03 ) 3==- C02 (c03 ) 3==- Hyp02C03- Np02+ H	<pre>8.31932E-01 9.96382E+00 5.61002E+00 6.1071E-03 1.11706E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.74407E-08 1.33846E-07 3.12502E-09 3.06048E-11 1.57050E-10</pre>	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.5850E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.8505E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.1933E-10 1.57050E-10	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000	1.93627E+01 3.47561E+00 1.95691E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.65762E-06 1.66368E-06 1.65484E-08 4.66887E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.47826E-11	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08022E-04 3.48446E-06 4.24701E-06 4.24701E-08 1.19831E-07 2.79779E-09 2.74002E-11 1.40605E-10
	H20 NaNpO2CO3(s) Na+ Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2+ H+ NpO2OH(aq) NpO2(OH)2-	NaNp02C03 ( s) Na+ C1- C03= HC03- OH- Np02 (C03) 2=- Np02 (C03) 3=- C02 ( aq) Np02 (C03) - H Np02 (C03) 2=- Np02 (C03) 2=- Np02 ( aq) Np02 (OH) 2-	8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 4.74407E-08 1.33846E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-12	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.0141E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.65682E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.47826E-13	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.66763E-03 1.00009E-03 1.08122E-04 3.88446E-06 4.27001E-06 4.27001E-06 4.2701E-06 4.2731E-07 1.9831E-07 2.79779E-09 2.74002E-11 1.40605E-10 1.49310E-12
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(ag) NpO2CO3- NpO2+ H+ NpO2OH(ag) NpO2(OH)2- Na3H(CO3)2.2H2O	NaNp02C03 (s) Na* C1- C03= HC03- OH- Np02 (C03) 3==- C02 (aq) Np02(C3) 3==- C02 (aq) Np02C03- Np02C03- H+ Np02C04 (aq) Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np02(OH)2- Np	<pre>8 31932E-01 9 96382E+00 5 61002E+00 6 1071E-03 1 11706E-03 1 20768E-04 3 89199E-06 4 76942E-06 4 76942E-06 4 3846E-07 3 12502E-09 3 06048E-11 1 57050E-10 1 66775E-12 0 00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5642 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65484E-08 4.66887E-08 4.66887E-08 1.09708E-09 1.06757E-11 5.81743E-13 0.00000E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.27001E-06 4.2701E-06 1.19831E-07 2.79779E-09 2.74002E-11 1.40605E-10 1.9310E-12 0.00000E+00
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2CA+ H+ NpO2(DK)2- Na3H(CO3)2.2H20	NaNp02C03(s) Na+ C1- C03= HC03- OH- Np02(C03)2=- Np02(C03)3=- C02(aq) Np02(c03) Np02(aq) Np02+ H+ Np02OH(aq) Np02(OH)2- Trona Thermonatrite	<pre>8.31932E-01 9.96382E+00 5.61002E+00 6.1071E-03 1.11706E-03 1.20768E-04 3.89199E-06 4.76942E-05 4.74407E-08 1.33846E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-12 0.0000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000	1.93627E+01 3.47561E+00 1.95691E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65484E-08 4.66887E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.47826E-11 5.47826E-11 5.81743E-13 0.0000E+00	4.96963E+01 8.92050E+00 5.0259E+00 5.01051E+00 5.06763E-03 1.08122E-04 3.48446E-06 4.2701E-06 4.24731E-08 1.19831E-07 2.79779E-09 2.74002E-11 1.40605E-10 1.49310E-12 0.00000E+00
	H20 NaNpO2CO3(s)Na+ Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2+ H+ NpO2(OH)2- Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)Na2CO3(H20)(H20)(H20)(H20)(H20)(H20)(H20)(H20)	NaNp02C03(s) Na+ Cl- C03= HC03- OH- Np02(C03)2=- Np02(C03)3=- C02(aq) Np02(c03)3=- C02(aq) Np02(c03)- Np02C03- Np02C03- Np02+ H+ Np02(0H)2- Thermonatrite L2C03-Heptahydrate	8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 4.74407E-08 1.33846E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-12 0.00000E+00 0.00000E+00	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01418E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.9335E-10 1.57050E-10 4.97826E-13 1.0000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 1.95220E+00 3.89655E-04 4.21267E-05 1.66368E-06 1.65368E-06 1.65484E-08 4.6688TE-08 1.09008E-09 1.06757E-11 5.47826E-11 5.47826E-11 5.81743E-13 0.0000E+00 0.0000E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.0009E-03 1.08122E-04 3.88446E-06 4.27001E-06 4.27001E-06 4.2701E-06 4.24731E-07 2.79779E-09 2.74002E-11 1.40605E-10 1.49310E-12 0.00000E+00 0.00000E+00
90090000000000000000000000000000000000	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2+ H+ NpO2(OH)2- Na3H(CO3)2.2H20Na Na2CO3.H20Na	NaNp02C03(s) Na* Cl- C03= HC03- OH- Np02(C03)3==- C02(aq) Np02c03)3==- C02(aq) Np02c04 Np02c04 Np02C04 Np02C04)2- Trona Thermonatrite L2C03-Heptahydrate	<pre>8 31932E-01 9 96382E+00 5 61002E+00 5 59653E+00 6 10711E-03 1 11706E-03 1 20768E-04 3 89199E-06 4 74407E-08 1 3386E-07 3 12502E-09 3 .06048E-11 1 57055E-10 1 66773E-12 0 .0000E+00 0 .0000E+00 0 .0000E+00</pre>	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.65368E-06 1.66368E-06 1.66368E-06 1.66368E-08 1.09008E-09 1.06757E-11 5.47026E-11 5.81748E-13 0.00000E+00 0.00000E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.2701E-06 4.2701E-06 4.24731E-08 1.19831E-07 2.79779E-09 2.74002E-11 1.40605E-10 1.49310E-12 0.0000E+00 0.00000E+00
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2+ H4 NpO2(OH(aq) NpO2(OH)2- Na3H(CO3)2.2H20Na2CO3.H20Na2CO3.H20Na2CO3.10H20Na Na2CO3.10H20Na	NaNpO2CO3(s) Na+ Cl- CO3= NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3) NpO2(C)3 NpO2(C)3- NpO2(H)2- Tromatrite 12CO3-Heptahydrate Natron Nahcolite	<pre>8 31932E-01 9 96382E+00 5 61002E+00 6 1071E-03 1 11706E-03 1 .20768E-04 3 .89199E-06 4 .76492E-06 4 .76492E-06 4 .76407E-08 1 .3846E-07 3 .12502E-09 3 .06048E-11 1 .57050E-10 1 .66773E-12 0 .00000E+00 0 .00000E+00 0 .0000E+00 0 .00000E+00</pre>	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.47826E-11 5.47826E-11 5.47426E-13 0.00000E+00 0.00000E+00 0.00000E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.27001E-06 4.2701E-08 1.19831E-07 2.79779E-09 2.74002E-11 1.40605E-10 1.49310E-12 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s) Na+ Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2+ H+ NpO2(OH)2- Na2CO3- NpO2(OH)2- Na2CO3(7H20Na Na2CO3(10H20Na NaClNaClNa	NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(C)3 NpO2CO3- NpO2+ H+ NpO2OH(2- Trona Trona Trona Trona Trona Trona Natron Natron Halice	<pre>8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 4.74407E-08 1.33846E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.9335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 1.95220E+00 3.89655E-04 4.21267E-05 1.65682E-06 1.65682E-06 1.65684E-08 1.09008E-09 1.06757E-11 5.47826E-13 5.81743E-13 0.0000E+00 0.0000E+00 0.0000E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.0009E-03 1.08122E-04 3.48446E-06 4.27001E-06 4.27001E-06 4.2701E-06 4.24731E-07 2.79779E-09 2.74002E-11 1.40605E-10 1.49310E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2+ H+ NpO2(OH)2- Na3H(CO3)2.2H20Na Na2CO3.10H20Na Na2CO3.10H20Na Na2CO3.10H20Na	NaNpO2CO3(s) Na* Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2(CO3)3==- CO2(aq) NpO2(CO3)2=- NpO2(A)2- NpO2(HQ1)2- Thermonatrite Natron Natron Natron Natron Natron Natron	<pre>8.31932E-01 9.96382E+00 5.61002E+00 5.59653E+00 6.1071E-03 1.11706E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.74407E-08 1.33846E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3598 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.81742E-13 0.00002E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.2701E-06 4.24731E-08 1.19831E-07 2.79779E-09 2.74002E-11 1.40605E-10 1.49310E-12 0.0000E+01 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2+ H4 NpO2(OH)2- Na3H(CO3)2.2H20 Na2CO3.7H20Na Na2CO3.7H20Na Na2CO3.10H20Na NaCO1NaSNpO2(CO3)2(s)NaCH(aq)to	NaNpO2CO3(s) Na+ Cl- CO3= NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2(CO3) NpO2(CO3)- NpO2(Aq) NpO2(CH)2- Tromonatrite 2CO3-Heptahydrate Nahcolite Nahcolite DISABLED_DISABLED Litrate.base.only	<pre>8 31932E-01 9 96382E+00 5 61002E+00 5 59653E+00 6 1071E-03 1 11706E-03 1 20768E-04 3 89199E-06 4 76492E-06 4 76492E-06 4 74407E-08 1 33846E-07 3 12502E-09 3 06048E-11 1 57050E-10 1 66773E-12 0 00000E+00 0 00000E+00 0 00000E+00 0 00000E+00 0 00000E+00</pre>	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65388E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.47826E-11 5.47826E-11 5.47826E-11 5.81743E-13 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.27001E-06 4.2701E-08 1.19831E-07 2.74072E-11 1.40605E-10 1.49310E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2(CO3)2=- NpO2(A)2- Na2CO3- Na2CO3- Na2CO3(CO3)2(s)_ NaCO3(20)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(S)2(s)_ Na3NpO2(S)2(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_	NaNpO2CO3(s) Na* Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- NpO2(CO3)2=- NpO2(A)32=- NpO2(A)32=- NpO2(A)32=- NpO2(A)32=- NpO2(A)32=- NpO2(A)32=- Natron Natron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron Katron KATron KATron KATron	<pre>8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 4.76942E-06 4.76942E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.0000E+00 1.00000E+00 1.00000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 1.95220E+00 3.89655E-04 4.21267E-05 1.65368E-06 1.65368E-06 1.65368E-06 1.65368E-08 1.09008E-09 1.06757E-11 5.47626E-13 5.47626E-13 5.81743E-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	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.0009E-03 1.08122E-04 4.27001E-06 4.27001E-06 4.27701E-06 4.27701E-07 2.79779E-09 2.74002E-11 1.40605E+10 1.49310E-12 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2(CO3)2=- NpO2(A)2=- NaD(2)2=- NaD(2)2=- Na3H(CO3)2(2)2=- Na3H(CO3)2(2)2=- Na2CO3(10H20Na)Na2CO3(10H20Na)Na2CO3(10H20Na)Na2CO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)NaCO3(10H20Na)Na)Na)NaCO3(10H20Na)Na)Na)Na)Na)Na)Na)Na)Na)Na)Na)Na)Na)N	NaNpO2CO3(s) Na* Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2CO4(apcd) NpO2OH(apcd) NpO2OH(apcd)	<pre>8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.1071E-03 1.11706E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.74407E-08 1.33846E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.81742E-13 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.2701E-06 4.24731E-08 1.19831E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74002E-11 1.40605E-10 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00
993 000 990 991 000 000 000 000 000 000 000	H20 NaNpO2CO3(s) Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2(CO3)2=- NpO2(A)2- Na2CO3- Na2CO3- Na2CO3(CO3)2(s)_ NaCO3(20)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(CO3)2(s)_ Na3NpO2(S)2(s)_ Na3NpO2(S)2(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_{S}(s)_	NaNpO2CO3(s) Na* Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2CO4(apcd) NpO2OH(apcd) NpO2OH(apcd)	<pre>8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 4.76942E-06 4.76942E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-12 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.0000E+00 1.00000E+00 1.00000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00 1.0000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 1.95220E+00 3.89655E-04 4.21267E-05 1.65682E-06 1.65682E-06 1.65684E-08 1.09008E-09 1.06757E-11 5.47826E-13 5.47826E-13 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.0009E-03 1.08122E-04 4.27001E-06 4.27001E-06 4.27701E-06 4.27701E-07 2.79779E-09 2.74002E-11 1.40605E+10 1.49310E-12 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s)Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO4(aq) NpO2(OH)2- Na2CO3(H20Na2CO3(H20Na2CO3(H20Na2CO3(H20Na2CO3(H20Na2CO3(H20Na2CO3(H20Na2CO3(H20(H20)(A))))))) Na2CO3(H20(H20(H20)(A)))) Na2CO3(H20(H20(H20)(A)))) Na2CO3(H20(H20(H20)(A)))))) Na2CO3(H20(H20(H20)(A)))))))))))))))))))))))))))))))))))	NaNpO2CO3(s) Na+ CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3) NpO2(CO3) NpO2(CO3)- NpO2(Aq) NpO2(H)2- Trona Thermonatrite L2CO3-Heptahydrate Natron Natron Natron Natroi titrate.base.only NpO2OH(amor) NpO2OH(amor) NpO2OH(aged).	<pre>8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 4.76942E-06 4.76942E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-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 0.00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.81742E-13 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.2701E-06 4.24731E-08 1.19831E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74002E-11 1.40605E-10 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s) Na+ Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- Na2CO3- NpO2(CO3)2=- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- Na2CO3- 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	H20 NaNpO2CO3(s)Na CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2+ H+ NpO2(OR)2- Na3H(CO3)2.2H20 Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NaC1NA NA NA NA NA NA NA NA NA NA NA NA NA N	NaNpO2CO3(s) Na+ Cl- CO3= NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2(CO3)- NpO2(CO3)- NpO2(CO3)- NpO2(CO3)- NpO2(CO3)- NpO2(CO3)- NpO2(CO3)- 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	H20 NaNpO2CO3(s)Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO3- NpO2CO4(aq) NpO2(OH)2- Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na2CO3.10H20Na+ Na+ Na2CO3.10H20Na+ Na+ Na+ Na+ Na+ Na+ Na+ Na+ Na+ Na+	NaNp02C03(s) Na+ C1- C03= HC03- OH- Np02(C03)2=- Np02(C03)2=- Np02(C03)3=- C02(aq) Np02(C03) Np02(C03) Np02(C04)2- Trona Thermonatrite L2C03-Heptahydrate Natron Natron Natron Natroi Litrate.base.only Np02OH(amor) Np02OH(aged) titrate.acid.only = 9.9232 ent= 1.240766	<pre>8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 4.76942E-06 4.76942E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-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 0.00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.81742E-13 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.2701E-06 4.24731E-08 1.19831E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74002E-11 1.40605E-10 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s)Na+ Cl- CO3= OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2+ H+ NpO2(OK)2- Na3CO3,2,2H20Na Na2CO3,7H20Na Na2CO3,7H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20Na Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA Na2CO3,10H20NA NA NA2CO3,10H20NA NA NA2CO3,10H20NA NA NA2CO3,10H20NA NA NA NA NA NA NA NA NA NA NA NA NA N	NaNpO2CO3(s) Na+ Cl- CO3= NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3)3=- CO2(aq) NpO2CO3- NpO2CO3- NpO2CO4 MpO2(H(aq) NpO2(H)2- Troma Thermonatrite L2CO3-Heptahydrate Mahcolite Halite DISABLED_DISABLED titrate.base.only NpO2OH(amor) NpO2OH(aged) titrate.acid.only = 9.9232 ent= 1.240746	<pre>8.31932E-01 9.96382E+00 5.61002E+00 5.9653E+00 6.10711E-03 1.20768E-04 3.89199E-06 4.76942E-06 4.76942E-06 4.76942E-06 4.76942E-07 3.12502E-09 3.06048E-11 1.57050E-10 1.66773E-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 0.00000E+00</pre>	7.78290E-01 1.00000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.81742E-13 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.2701E-06 4.24731E-08 1.19831E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74703E-07 2.74002E-11 1.40605E-10 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00
	H20 NaNpO2CO3(s)Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2+ H+ NpO2(OH)2- Na3H(CO3)2.2H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na NaCH(aq)to NpO2OH(aged)Na NaOH(aged)Na NaOH(aged)ND NaOH(aged)ND NpO2(M(aged) HC1(aq)to NpM = -log(a(H+)) Osmotic Coefficie Equilibrium RH (4	NaNp02C03(s) Na+ Cl- C03= Np02(C03)2=- Np02(C03)3=- C02(c03)3=- C02(c03)3=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Np02(C03)2=- Natoria Np02(C03)2=- Natoria Natoria Natoria Np02(C03)2=- Natoria Natoria Np02(C03)2=- Natoria Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria Np02(C03)2=- Natoria 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1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.81742E-13 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 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	H20 NaNpO2CO3(s)Na CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2CO3- NpO2+ H+ NpO2(OR)2- Na3H(CO3)2.2H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na NaC1Na Na NoTES: - Water	NaNp02C03(s) Na+ C1- C03= HC03- OH- Np02(C03)2=- Np02(C03)2=- Np02(C03)3=- C02(aq) Np02(C03) H+ Np02(C04)2- Trona Trona Trona Trona Trona Trona Trona Trona Trona Trona Trona Trona Trona Np02(H(aq) Np02(H(aq) DISABLED_DISABLED DISABLED_DISABLED_DISABLED_DISABLED_DISABLED_DISABLED_DISABLED_DISABLED_DISABLED_DISABLED_I Np02OH(agod) titrate.acid.only = 9.9232 ent= 1.240746 N) = 77.828965 n) = 5.616187 = 1188.79	<pre>8 31932E-01 9 96382E+00 5 61002E+00 5 59638E+00 6 1071E-03 1 11706E-03 1 20768E-04 3 89199E-06 4 7407E-08 1 3386E-07 3 12502E-09 3 .06048E-11 1 57050E-10 1 66773E-12 0 .0000E+00 0 .00000E+00 0 .00000E+00 1 .0000E+00 0 .00000E+00 0 .00000E+00 1 .0000E+00 0 .00000E+00 0 .00000E+00 1 .0000E+00 0 .0000E+00 0 .00000E+00 0 .0000E+00 0 .00000E+00 0 .00000E+00 1 .0000E+00 0 .000</pre>	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000	1.93627E+01 3.47561E+00 1.95591E+00 2.13030E-03 3.89655E-04 4.21267E-05 1.35762E-06 1.65368E-06 1.65484E-08 4.66887E-08 1.09008E-09 1.06757E-11 5.81742E-13 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.000	4.96963E+01 8.92050E+00 5.02259E+00 5.01051E+00 5.46763E-03 1.08029E-03 1.08122E-04 3.48446E-06 4.27001E-06 4.24731E-08 1.19831E-07 2.74709E-09 2.74002E-11 1.40605E-10 1.49310E-12 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
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C1- C03= HC03- OH- Np02(C03)2=- Np02(C03)2=- Np02(C03)3=- C02(aq) Np02(C03) Np02(C03) Np02(C03) Np02(C04)2- Trona 	<pre>8 31932E-01 9 96382E+00 5 61002E+00 5 59638E+00 6 1071E-03 1 11706E-03 1 20768E-04 3 89199E-06 4 7407E-08 1 3386E-07 3 12502E-09 3 .06048E-11 1 57050E-10 1 66773E-12 0 .0000E+00 0 .00000E+00 0 .00000E+00 1 .0000E+00 0 .00000E+00 0 .00000E+00 1 .0000E+00 0 .00000E+00 0 .00000E+00 1 .0000E+00 0 .0000E+00 0 .00000E+00 0 .0000E+00 0 .00000E+00 0 .00000E+00 1 .0000E+00 0 .000</pre>	7.78290E-01 1.0000E+00 5.28628E+00 5.27166E+00 1.58505E-04 4.13103E-04 6.57227E-05 1.01411E-10 3.85055E-15 1.37761E-07 2.43265E-07 6.18962E-09 1.19335E-10 1.57050E-10 4.97826E-13 1.0000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.9355 1.000 0.9423 0.9420 2.5954E-02 0.3698 0.5442 2.6056E-05 8.0734E-10 2.904 1.817 1.981 3.899 1.000 0.2985 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000 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	H20 NaNpO2CO3(s)Na+ Cl- CO3= HCO3- OH- NpO2(CO3)2=- NpO2(CO3)3==- CO2(aq) NpO2CO3- NpO2+ H+ NpO2(CO3)2.2H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na Na2CO3.H20Na NaCH(aq)to NpO2OH(aged) NpO2OH(aged) NpO2OH(aged) NpO2OH(aged) NpO2OH(aged) NpO2OH(aged) NDOTES: - Water ^ Gas *mc - Cos *mc - Cos *mc - Cos *mc	NaNpO2CO3(s) Na+ Cl- CO3= NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)2=- NpO2(CO3)3=- CO2(aq) NpO2(CO3) NpO2(CO3) NpO2(CO3) NpO2(CO3) NpO2(CO3) NpO2(CO3) NpO2(CO3) NpO2(CO3) NpO2CO3- NpO2CO4(aq) NpO2(CO3) NpO2(CO3) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) NpO2CO4(aq) 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DmH = -log(m(H+)) DH = -log(m(H+)) DH = -log(m(H+)) DFM = -log(m(H+)) DFM = -log(m(H+)) Comotic Coefficie Equilibrium RH (& Ionic Strength (m Density, kg/m3) NOTES: - Water * - Gas *mc - *Descri *GG/RT/_	NaNp02C03(s) Na+ Cl- C03= Np02(C03)2=- Np02(C03)3=- C02(aq) Np02(C03)3=- C02(aq) Np02(C03)3=- C02(aq) Np02(C03)3=- C02(aq) Np02(C03)3=- C02(aq) Np02(C03)3=- C02(aq) Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- Np02(C03)3=- 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*log10(partial pressure) for gases

409 440 -4.64192502E+03 Total G/RT=

TITRATE file name is U1: {SCBABB.FMT.USERGUIDE}NP_NACL_EM_LIN.TITRATE;2 263

.

Appendix O: Sample Output File "Np_NaCl_BM_LIN.OUT"

443 MOLES file name is U1: (SCBABB.FMT.USERGUIDE)NP_NACL_BM_LIN.MOLES;1



INFUT 2

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

### Appendix P: Sample Output File "Np_NaCl BM.OUT"

#### See Table 27 for explanation of this listing. file name is U1: (SCBABB.FMT.USERGUIDE)NP_NACL_BM.IN; 1 INGUESS file name is U1: [SCHABB.FMT.USERGUIDE]NP_NACL_BM.INGUESS:1 file name is U1: [SCBABB.FMT.USERGUIDE]NP_NACL_BM.OUT;1

OUTPUT CHEMDAT file name is U1: [SCBABB.FMT.USERGUIDE] FMT_HMW_NP_AM.CHEMDAT: 1 Temperature is Hard Coded as 298.15K ċ Benchmark TITRATE Problem; Np(V)02 with CO3 in 5.61molal NaC1 FMT V2.0 Benchmark fileRic FiR85; Np(V)-Na-C03-OH-C1-C104 (NR94); DATABASE: H5M84/FW85; Np(V)-Na-C03-OH-C1-C104 (NR94); 95.01.31 Am(III)-Na-C1-C03-S04-P04 (FRSR89,FRF90,F91,RFFR92,RFF94,RRFF94) _____ "2 *** ECHO PRINT OF "CHEMDAT" FILE WOULD BE HERE *** ... SEE APPENDIX J *** ۰,۰ ....... TITRATION Problem -) Assigning all delta(y) to 0.1 m -) Setting # of nodes in Y-direction to 3 -) Setting NONREACTIVE Porosity to 0.0 1 1 Specifying VARIABLE POROSITY for TITRATION Problem 24 23  $\frac{2}{2}$   $\frac{2}{2}$  Aqueous Density is a Function of Composition 11 RHOMIN file name is U1: [SCBABB.FMT.USERGUIDE] FMT_HMM_NP_AM.RHOMIN; 1 21 20 20 *** TABLE OF MINERAL DENSITIES, KG/M^3 WOULD BE HERE *** ... SEE APPENDIX L GRID BLOCK VOLUMES, in liters 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 20 1.00E+00 1.00E+00 22 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00 1.005+00  $c_{2}$ 23 1.00E+00 1.00E+00 17 1.002+00 1.002+00 1.002+00 1.002+00 1.002+00 1.002+00 1.002+00 1.002+00 1.002+00 1.002+00 1.002+00 1.002+00 -0 1.00E+00 1.00E+00 4 4.5 :5 # inversions for batch pblm 50 47 IBenchmark TITRATE Problem; Np(V)02 with CO3 in 5.61molal NaCl FMT V2.0 ∴ iDericimers litrate Projem; Np(V)/02 With CO3 in 5.81mOlal NaCl 43 DaTABASE: H9M84/FW86; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94); 43 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94) 2 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin 5 Elemental Abundances for Flash Problem 5.1 57 Aq. Molarity Ag. mg/liter Total Moles Ag. Molality  $\dot{\gamma} \in \dot{\gamma}$ 1.11017363E+02 1,11029658E+02 1.00100314E+02 1.00891107E+05 Hydrogen 8.87328944E+05 5,54601388E+01 6.15086815E+01 6.15154934E+01 Oxygen 1.16289907E+05 5.61000000E+00 5.610621292+00 5.05833276E+00 Sodium 5. 50 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.00000002+00 Potassium 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 10 Magnesium 0.0000000E+00 0.00000002±+00 0.0000000E+00 0.0000000E+00 Calcium 6.7 1.61000000E+00 1.61017830E+00 1.45167838E+00 5.14663538E+04 Chlorine 0.00000000E+00 0.000000002+00 0.0000000E+00 0.00000000E+00 ÷0 Sulfur ş. 2.00000001E+00 2.000221502+00 1.80332719E+00 2.16597629E+04 Carbon 0.0000000E+00 0.0000000E+00 0 0000000E+00 0.000000005+00 Posion 1.1. 0.0000000E+00 0.0000000E+00 €€ 0.0000000E+00 0.00000000E+00 Negion 0.0000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Air £8 44 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.00000000E+00 Boron 0.0000000E+00 0.00000000E+00 0.0000000E+00 0,0000000E+00 Bromine 0.00000000000000 Q.0000000E+00 0.0000000E+00 0.0000000E+00 TracerEl 0.0000000E+00 0 00000000E+00 Q.00000000E+00 0.000000005+00 Th(IV) 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Am(III) 72  $\mathbb{T}^{2}$ 0.0000000E+00 ٥ .0000000E+00 0.0000000E+00 0.00000000E+00 U(VI) 0.00000000E+00 0.0000000E+00 Ξ. 0 0000000E+00 ND(V) 25 0.000000002+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 C104-(EL) 0.0000000E+00 0.00000002+00 0.0000000E+00 0.00000000E+00 Phosphorus 20 77 0.0000000E+00 0.0000000E+00 0.00000000E+00 0.0000000E+00 Electron -2.22044605E-15 -2.22069196E-15 -2.00209536E-15 0.0000000E+00 73 Charge 24 2.2 Solution Parameters, Calculated SOLUTION MASS 1306.07033909890 grams H20 MASS 999.889265717486 8." grams

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Appendix P: Sample Output File "Np_NaCl_BM.OUT"

306.214981877726 TDS (g/kg) g/kgH20 34 94 Specified Solution Density 1177.63607439302  $kg/m^3 = g/1$ 64 DENSITY ÷ r Solution Parameters Based on Specified Density 1.10906108219560 SOLUTION VOL. liters 8.4 30 TDS 276.072326670473 g/1 42 Density based on TDS and NaCl solutions 1177.63607439302 q/1 Percent relative error vs NaCl density 0.000000000000000000000 14 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM e è Species Name Molality Activity Act Coef Total Moles Molarity mg/liter Descriptor :01 - 14 WATER 8.57464E-01 8.59843E-01 1.003 5.55025E+01 5.00446E+01 H20 9.01564E+05 9 9 9 5.61062E+00 1.99407E+00 3.69881E+00 0.6593 5.61000E+00 5.05833E+00 1.16290E+05 Na+ Na+ 4.09214E-02 C03= CO3= 2.0522E-02 1.99385E+00 1.79778E+00 1.078846+05 **c**1-1.61018E+00 1.06477E+00 0.6613 1.61000E+00 1.45168E+00 5.14664E+04 C1-6.14734E-03 6.14733E-03 нсоз-HCO3-1.59044E+03 0.2587 6.14666£-03 5.54222E-03 3.38170E+02 4 86901E-03 0H-OH-0.7921 6.14665E-03 5.54221E-03 9 42580E+01 2.00E-11 CO2 (aq) 2.36876E-09 2.36850E-09 2.13559E-09 9.39868E-05 2.2C02 (ag) 7.15913E-09 3.022 -2.12E-07 1.77959E-12 - 4. H+ H+ 2.39954E-12 0.7416 2.399272-12 2.16334E-12 2.18043E-09 -8.58E-08 109 Na3H (CO3) 2.2H20_ 0.00000E+00 Trona 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -1.57E+00 HC1(ag).....to.titrate.acid.only 1.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 ~2.52E+02 NaOH(ag).....to.titrate.base.only 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.92E+02 _____Halles 0.00000E+00 1.00000E+00 1,000 0.00000E+00 0.00000£+00 0.00000E+00 NaC1 -9.75E-01 . . . NaHCO3 0.00000E+00 0.00000E+00 1.00000£+00 1,000 0.00000E+00 0.00000E+00 -1,83E+00 Na2CO3 7H20 Na2CO3-Heptahydrate 0.00000E+00 1 00000E+00 1.000 0.00000E+00 0 00000E+00 0.00000E+00 -2.51E-01 0.00000E+00 0.00000E+00 1.000 Na2CO3.H20_____Thermonatrite 1,00000E+00 0.00000E+00 0.00000E+00 -7.998-01 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -8.30E-02 117 ``f pmH = -log[m(H+)]
`` / pH = -log[a(H+)] 11.6199 pH = -log[a(H+)]11.7497 Osmotic Coefficient= 0.908418 Equilibrium RH (%) = 85.984284 22 Ionic Strength (m) = 7.604695 = 1177.64 978 Density, kg/m3 NOTES: - Water 'molality' is mole fraction H2O in aqueous phase - Gas 'molality' and 'activity' are gas partial pressures - 'Descriptor' means: 20 :23 *dG/RT/ln10 for species with nonzero concs. (convergence criterion) 120 *Saturation Index for minerals, SI=log10(IAP/Ksp) *log10(activity) for aqueous species with very small concentrations :30 *log10(partial pressure) for gases Total G/RT# -6.42133776E+03 34 2. 2.000000000000000 Reaction # l sldsum 2 This is a solid-only reaction - ....v shifting left by 4.64434654478256 calling makenuv for allomorphic reactions 150 # inversions for batch pblm 75 19 1Benchmark TITRATE Problem; Np(V)02 with CO3 in 5.61molal NaCl FMT V2.0 DATABASE: MONGAT/FWG6; Np(V)-Na-CO3-OH-Cl-ClO4 (NR94); 95.01.31 An(III)-Na-Cl-CO3-SO4-PO4 (FRSR89, FRF90, P91, RFFR92, RFF94, RRFF94) 140 ..... 1.00000E+00 [=] ATM 2.98E+02 [=] Kelvin Pressure* Temperature= .... •40 Elemental Abundances for Flash Problem' 16 : 65 Total Moles Aq. Molality Aq. Molarity Ag. mg/liter °43.3 16-2 1.110183635+02 1.11017591E+02 9.93638668E+01 1.00169020E+05 Hydrogen :0 :2 4.96942389E+01 5.02263316E+00 1.05508682E+02 5.55113597E+01 7.95078006E+05 Oxygen 1.15469181E+05 1.56100000E+01 5.61057382E+00 Sodium • 82 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Potassium - 1. 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 Magnesium - 46 0.0000000E+00 0.0000000E+00 0.0000000E+00 Calcium 150 5.02297975E+00 5.61100000E+00 5.61096098E+00 1.78079701E+05 Chlorine 0.00000000E+00 6.12839261E-04 0.0000000E+00 6.58946152E+00 0.00000002+00 0.0000000E+00 Sulfur 5.48618892E-04 1.0000000E+01 Carbon 165 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Posion 0.00000000£+00 0.0000000E+00 0.0000000E+00 NegIon ÷., 0.0000000E+00 0.00000000E+00 0.00000000E+00 0.0000000E+00 Air **م**ج، 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Boron 101 101 101 0.0000000E+00 0.00000000E+00 0.00000002+00 Bromine 0.000000002+00 0.0000000E+00 0.000000000000 0.0000000E+00 TracerEl 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Th(IV) - 5.2 0.00000000E+00 0.00000000E+00 0.00000000E+00 Am(III) 0.000000002+00 27 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.00000000E+00 U(VI) 1985 1.0000000E+01 6.12839261E-04 0.00000000E+00 5.48618892E-04 1.30049121E+02 No (V) 101 0.0000000E+00 0.0000000E+00 0.0000000E+00 Cl04-(EL) 170 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Phosphorus 0.0000000Eton 0.00000000000000 0.00000000000+00 0.00000005+00 Electron -2.37316632E-15 -2.37314981E-15 -2.12446380E-15 0.0000000E+00 Charge

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73	Solution Paramete	we Calculated							
.7:	SOLUTION MASS	1328.11614865142	2 grams						
170	H20 MASS	1000.0069546681							
177	TDS(g/kg)	328.106912108529	-						
$\frac{1}{7}$			• •.						
	Specified Solution	on Density							
560	DENSITY	1188.9325460547	7 kg/m^3 =	g/l					
131									
22		ers Based on Specif							
2.	SOLUTION VOL	1.1170660211620							
154. 	TDS	293.72408413418	7 g/l						
140		TDS and NaCl solut		254605477	g/l				
· · ·		error vs NaCl dens		0000000000E+000	-				
120	Percent relative		,						
18.1									
14.3									
÷ .	TABLE OF CONCENTRAT	TIONS FOR BATCH SYS	STEM						
7 v.)									
	Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
104	H2O		0 210228-01	7 770505-01	0.9352	5.55091E+01	4 969195.03	0.050000.05	
		WATER	8.31822E-01 9.99932E+00	7.77959E-01 1.00000E+00	1.000	9.99939E+00	4.96918E+01 8.95147E+00	8.95208E+05 3.15133E+06	
	NaNp02C03(s)	NaNpO2CO3(s) C1-	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)	C02 (ag)	3.86103E-04	1.12115E-03	2.904	3.86106E-04	3.45643E-04	1.52117E+01	
	нсоз-	HCO3-	2.26571E-04	8.38810E-05	0.3702	2.26573E-04	2.02829E-04	1.23760E+01	4.26E-09
202	Np02C03-	Np02C03-	1.33526E-07	2.42971E-07	1.820	1.33527E-07	1.19534E-07	3.93334E-02	-1.99E-11
203		H+	1.21872E-06	4.78095E-06	3.923	1.218732-06	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	4.59318£-05	2.55E-08
	NpO20H (aq)	NpO20H(ag)	7.72186E-10	7.72186E-10	1.000 2.5877E-05	7.72191E-10	6.91267E-10	1.97740E-04 6.90960E-06	1.872-07
	NpO2 (CO3) 2=- NpO2 (OH) 2-	NpO2 (CO3)2=- NpO2 (OH)2-	1.98384E-11 2.04382E-16	5.13354E-16 6.10703E-17	0.2988	1.98385E-11 2.04383E-16	1.77595E-11 1.82964E-16	5.54494E-11	-1.62E-07 2.13E-07
	Np02 (CO3) 3==-	NpO2 (CO3) 3==-	1.25197E-16	9.87896E-26	7.8908E-10	1.251982-16	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
211			0.00000E+00	0.00000£+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.99E+02
012	HCl(aq)to.ti		0.00000E+00	0.0000E+00	1.000	0.00000E+00	0.00000E+00	0.0000E+00	-2.45E+02
212	Na3Np02(C03)2(s)_D	SABLED_DISABLED	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.0000E+00	0.0000E+00	-9.36E+02
	NaCl	Halite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.0000E+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
	Na2CO3.10H20	Natron	0.00000E+00 0.00000E+00	1.00000E+00 1.00000E+00	1.000	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000±+00 0.00000±+00	-7.91E+00 -7.95E+00
	Na2C03.7H20Na2C Na2C03.H20Na2C		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.24E+00
	Na3H(CO3)2.2H20	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.02E+01
	NpO2OH(amor)		0.00000E+00	1.00000E+00	1.000	0.00000£+00	0.00000E+00	0.00000E+00	~2.98E+00
2.21		<u> </u>							
	pmH = -log[m(H+)]	<b>#</b>	5.9141						
	pH ≠ -log[a(H+)]	= 5.3205							
	Osmotic Coefficient								
	Equilibrium RH (%)								
	Ionic Strength (m) Density, kg/m3	= 5.611188 = 1188.93							
2.15	Densiey, Ny/ab								
	NOTES: - Water *mc	lality" is mole for	raction H2O in a	queous phase					
232		lity and activit							
23	<ul> <li>Descript</li> </ul>								
232		10 for species with			e criterion)				
2/3		on Index for mines							
254		tivity) for aqueon		very small con	entrations				
285	-Toâta (be	rtial pressure) fo	- yas <del>t</del> s						
	Total G/RT= -1.3	3323084E+04							
	Flashing Titration								
	# inversions for ba		11						
2.4	1Benchmark TITRATE F	roblem; Np(V)02 w:			1	FMT V2.0		•	
	DATABASE: HMW84/FW							, en	
	95.01.31 Am(III)-								· · ·
243 264	Pressure= 1		A Temperatu:	2.302+0	02 [=] Kelvin			ţ.	
	Elemental Abundance	s for Flash Proble	≥m.					р С	
2									
	Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter				×.	
043		-	-					,	
249			9.93838868E+01	1.00169020E+					,
250	3.66707638E+01		4.96942389E+01	7.95078006E+					
2*1	5.42543623E+00		5.02263316E+00 0.0000000E+00	1.15469181E+					
250 263	0.0000000E+00 0.0000000E+00		D.00000000E+00	0.00000000E+0					
200	0.0000000E+00		0.000000002+00	0.00000000E+0					
265			5.02297975E+00	1.78079701E+					
256	0.0000000E+00		0.0000000E+00	0.0000000E+					
257	3.47561578E+00		5.48618892E-04	6.58946151E+					
253	0.0000000E+00		0.0000000E+00	0.0000000E+					
289	0.00000000000000		0.0000000E+00	0.0000000E+					
000	0.0000000E+00		0.0000000E+00	0.0000000E+0					
201	0.0000000E+00		0.00000000E+00	0.00000000E+0					
262	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+(	AA DIANTUG				

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

16.3 0.0000000E+00 0.0000000E+00 TracerE1 0.0000000E+00 0 0000000E+00 0.00000000E+00 · . . 0 00000005+00 Th(IV) 0.0000000E+00 0.0000000E+00 20 0.0000000E+00 0.0000000E+00 Am(III) 000 70 743 0,00000000E+00 0.00000000E+00 0.0000000E+00 0.00000000000000 U(VI) 5.48618892E-04 1.30049121E+02 Np(V) 6 12839260E-04 3 47561578E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 C104-(EL) 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 Phosphorus 253 27.) 27 0.0000000E+00 0.0000000E+00 0.00000005+00 0.0000000F+00 Electron -6.94525850E-16 -1.99826754E-15 -1.78886601E-15 0.00000000E+00 Charge 
 Solution Parameters, Calculated

 SOLUTION MASS
 461.602144251012

 H20 MASS
 347.563995068956
 4... orams 275 275 274 grams TDS(g/kg) 328.106912108175 g/kgH20 194 197 Specified Solution Density 1188.93254605459  $kg/m^{3} = g/1$ DENSITY 26. 2.5 Solution Parameters Based on Specified Density liters ъ. SOLUTION VOL 0.388249228926247 ٢. 293.724084133903 TDS q/l 7188 93254605459 Density based on TDS and NaCl solutions g/1 Percent relative error vs NaCl density 0.000000000000000E+000 % 277 26.5 250 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM 2742 Species Name Activity Act Coef Total Moles Molarity Molality mg/liter Descriptor 29.³ 8.31822E-01 7.77959E-01 0.9352 244 120 WATER 1.92928E+01 4.969182+018.95208E+05 206 NaNp02C03 (s)_ _NaNpO2CO3(s) 9.99932E+00 1.00000E+00 1.000 3.47540E+00 8.95147E+00 3.15133E+06 200 5 61096E+00 5.29329E+00 0.9434 1.95017E+00 5.02298E+00 1.78080E+05 C1-C1-Na+ Na+ 5.61057E+00 5.29268E+00 0.9433 1.95003E+00 5.02263E+00 1.15469E+05 1.2 Np02+ 1.21978E-03 2.12954E-04 5.48499E-04 ND02+ 6.12705E-04 1.991 1.47572E+02 2~3 CO2 (aq) C02 (ag) 3.86103E-04 1.12115E-03 2,904 1.34196E-04 3.45643E-04 1.52117E+01 .«Э нсоз-HC03-2 26571E-04 8.38810E-05 0.3702 7.87481E-05 2 02829E-04  $1.23760 \pm 01$ -6.17E-15 H+ 4.78095E-06 4.23582E-07 1.09101E-06 1.21872E-06 3.923 1.09962E-03 10 H+ 6.17E-15 Np02C03-202 Np02C03-1.33526E-07 2.429712-07 1.820 4.64090E-08 1.19534E-07 3.93334E-02 1.85E-14 302 co3= CO3= 3.09384E-08 8.03343E-10 2.5966E-02 1.07531E~08 2.769638-08 1.66203E-03 0.00E+00 1.63977E-09 OH-0.5435 1.04855E~09 2.70071E-09 3.01685E-09 4.59318E-05 -6.17E-15 OH-NpO20H(aq) 205 Np020H(aq) 7.72186E-10 7.72186E-10 1.000 2.68384E-10 6.91267E-10 1.97740E-04 0.00E+00 5.13355E-16 . US . US NpO2 (CO3) 2=-NpO2 (CO3) 2=-1.98384E-11 2.5877E-05 6.89511E+12 1 775958-11 6.90960E-06 0.00E+00 Np02 (0H) 2-6.10703E-17 7.10356E-17 2.04381E-16 0.2988 1.82964E-16 5.54494£-11 NoO2 (OH) 2-1.23E-14 Np02 (C03) 3==-Np02 (C03) 3==-1.251972-16 9.87897E-26 7.890BE-10 4.35139E-17 1.12077E-16 5.03310E-11 -3.53E-10 203 HCl(ag).....to.titrate.acid.only NpO2OH(aged)_____NpO2OH(aged) 25.2 0.00000E+00 0.00000E+00 1,000 0.00000E+00 0.00000E+00 0.00000E+00 -2.45E+02 ____NpO2OH(aged) ____NpO2OH(amor) 310 31 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.38E+00 NpO2OH (amor) 0.00000E+00 1.00000E+00 1.000 0.00000£+00 0.00000E+00 0.00000E+00 -2.98E+00 NaOH(aq)....to.titrate.base.only Na3NpO2(CO3)2(s)_DISABLED_DISABLED 0.00000E+00 0.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 -2.99E+02 1.00000E+00 0.000002+00 'n, 1,000 0.00000E+00 0.00000E+00 0.00000E+00 -9.36E+02 ______Halite 1.0 C.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00 -1.23E-01 NaCl 1.000 0.00000E+00 11.1 NAHCO3 0.00000E+00 1.000002+00 1.000 0.000008+00 0.00000E+00 0.00000E+00 -2.95£+00 Na2CO3.10H2O 1.00000E+00 1.000 0.00000E+00 Natron 0.00000E+00 0.00000E+00 0.00000E+00 -7.91E+00 2.00 Na2CO3.7H20____Na2CO3-Heptahydrate 1.00000E+00 0.00000E+00 0.00000E+00 -7.95E+00 0.00000E+00 1,000 0.00000E+00 _____Thermonatrite 15 Na2CO3 H20 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0 00000E+00 0 0000000+00 -8.24E+00 Na3H(CO3)2.2H20 0.00000E+00 1.00000E+00 1.000 0.00000E+00 0.00000E+00 0.00000E+00 Trona -1.02£+01 ..... 201 pmH = -log[m(H+)] 5.9141 5.3205 22 pH = -log[a(H+)]÷ Osmotic Coefficient= 1.241871 Equilibrium RH (%) = 77.795863 200 Ionic Strength (m) = 5.611188 320 Density, kg/m3 1188.93 32 22 NOTES: - Water "molality" is mole fraction H2O in aqueous phase - Gas 'molality' and 'activity' are gas partial pressures  $(\cdot, \cdot)$ 2.0 - "Descriptor" means: *dG/RT/lnl0 for species with nonzero concs. (convergence criterion) ..... *Saturation Index for minerals, SI#log10(IAP/Ksp) *log10(activity) for aqueous species with very small concentrations 32. *log10(partial pressure) for gases 52 20 2 -> Total G/RT= -4.63379813E+03 333 *** SUMMARY INFORMATION FOR ADDITION OF DV(2)...DV(14) WOULD BE HERE *** ÷4. Flashing Titration # 15 # inversions for batch pblm 22 34 IBenchmark TITRATE Problem; Np (V) 02 with CO3 in 5.61molal NaCl FMT V2.0 DATABASE: HMW84/FW86; Np(V)-Na-CO3-OH-Cl-Cl04 (NR94); 95.01.31 Am(III)-Na-Cl-CO3-SO4-PO4 (FRSR89,FRF90,P91,RFFR92,RFF94,RRFF94) . . . •...? 1.00000E+00 [=] ATM 2.98E+02 [=] Kelvin ي ينها Temperature= Pressure= 145 Elemental Abundances for Flash Problem 35 1000 Total Moles Aq. Molality Aq. Molarity Aq. mg/liter

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			≫4[0 <b>X</b> [410]	-	0000000000000 0000000000000 0000000000	۲۲ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲	473.2396423655 556.574003417592 227.465491025424 on Density 1188.6038311666549681 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350 293.210437350 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210500000000000000000000000000000000000	ΤΑΒLE ΟΓ CONCENTRA Percent relative Density based on Solution Peramet Solution Peramet Solution Peramet H2O PAGS Percent relative Percent relative
			24[0 <b>X</b> [410]	τ/	00000000E+000 ≇ 1383111842 č č\γ	TSK وتعید وتعید وتعید ریک ریک ریک ریک ریک ریک ریک ریک	ers, Calculated 473.339684533635 327.465491025424 on Density 1188.60383111845 593.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350 293.210437350 293.210437350 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.21000000000000000000000000000000000000	ΤΑΒLE ΟΓ CONCENTRA TABLE ΟΓ CONCENTRA Percent relative Solution Peramet Solution Peramet TDS Solution VOL TDS Solution VOL TDS Solution VOL TDS Solution Peramet Solution VOL TDS Solution VOL TDS Solution VOL Solution VOL
			24[0 <b>X</b> [410]	∖J CJP3T8€	0000000000000 0000000000000 0000000000	۲۲ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲	ers, Calculated 473.339684533635 327.465491025424 on Density 1188.60383111845 593.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350 293.210437350 293.210437350 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.21043750 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210437550 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.210450 293.21000000000000000000000000000000000000	ΤΑΒLE ΟΓ CONCENTRA TABLE ΟΓ CONCENTRA Percent relative Solution Peramet Solution Peramet TDS Solution VOL TDS Solution VOL TDS Solution VOL TDS Solution Peramet Solution VOL TDS Solution VOL TDS Solution VOL Solution VOL
			≫4[0 <b>X</b> [410]	\] Συστζε Γτοςτου	00000000000000000000000000000000000000	TSK وتعید وتعید وتعید ریک ریک ریک ریک ریک ریک ریک ریک	.5-134688/2112-15 -15 .ers, Calculated 472.139684531655 227.4654910247752 227.4654910247752 227.4654910347752 232.210437350984 233.210437350984 293.210437350984 293.210437350984 293.210437350984 293.210437350984	ΤΑΒLE ΟΓ CONCENTRA TABLE ΟΓ CONCENTRA Percent relative Solution Peramet Solution Peramet TDS Solution VOL TDS Solution VOL TDS Solution VOL TDS Solution Peramet Solution VOL TDS Solution VOL TDS Solution VOL Solution VOL
				∖J CJP3T8€	000000000E+000 # 1383111842 6 6\7 6\7	۲۸ ۲۸ ۲۸ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶	-5.12488071E-15 -5.12488071E-15 259.21043545165 -5.1204317592 227.204317592 227.2043171545 227.2043171545 227.2043171545 227.20437159542 227.20437159542 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.204371595 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.2045715 227.20457575 227.204575 227.2045755 227.2045755 227.20557	ΤΑΝΤΕ ΟΓ CONCENTRA TANLE ΟΓ CONCENTRA Solution Paramet Solution Paramet Solution Paramet TDS (9/99) TDS Solution Vol TDS Solution Vol T
			≫4[0 <b>1</b> [€10]	\] Συστζε Γτοςτου	00000000000000000000000000000000000000	۲۲ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶	0.00000000 0.00 0.000000000 0.00 0.0000000000	TABLE OF CONCENTRA           Percent relative           Density based on           Solution Por
			≫4[0 <b>X</b> [€10]	\]	00000000E+000 # 383111842 & & 3\\ 3\\ 3\\ 3\\ 3\\ 0\\ 0\\ 0\\ 0\\ 0\\	EX at 0.000000 at 1188.60 at 2000 by 2000 by 20000 comparish at 2000 comparish at 2000000 comparish at 2000 comparish at 2000 at 2000 a	0 0.00000002+00 0 0.0000002+00 0 0.0000002+00 0 0.0000002+055 0.00000002+055 0.00000002+055 0.00000002+055 0.00000002+055 0.000000005+05 0.00000000 0.00000005+05 0.00000000 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.00000005+00 0.000000000 0.000000000 0.00000000	TABLE OF CONCENTRA           Percent relative           Density based on           Solution Peramet           Solutintint           Solution Per
			24[0 <b>X</b> [410]	\] CJ93LG6 EJ962LOJ BD08D90LR5 CJ04-(ET)	000000005+000 # 393111842 5 5\7 5\7 0.000000500 00+300000000 00+300000000 00+300000000	۲۲ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶	2.881024985-04 2. 0.000000025-00 0. 223.210437325424 237.465491025424 237.4654910254234 237.4654910254234 237.4654910254234 237.4654910254234 237.4654910254234 237.4654910254234 237.200000005-00 0. 237.4654910254234 237.200000005-00 0. 237.4654910254234 237.200000005-00 0. 237.4654910254234 237.200000005-00 0. 237.200000005-00 0. 247.200000005-00 0. 259.210437350384 247.200000002-00 0. 259.210437350384 247.200000002-00 0. 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350384 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.210437350584 259.2104375555 259.2104375555 259.2104375555 259.2104375555 259.2104375555 259.2104375555 259.21043755555 259.2104375555 259.2104375555 259.2104375555 259.21043755555 259.210455555 259.2104555555 259.2104555555 259.210455555 259.210455555 259.2104555555 259.210455555555 259.210455555555555 259.2104555555555555555555555555555555555555	TABLE OF CONCENTRA           Pensity Descion           Pensity Descion           Solution Persmet           Solution Person           Solution Person           Solution Person           Solution Person           Solution Person           Solution
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				\J CJ93L36 EJ66L10J Lposbuoins CIO4-(EΓ) μβ(Δ) Ω(Δ1)	0000000000€00 1393117842 č 1393177842 č 1393177842 0 0.00000000€00 0.000000000 0.0000000€00 0.0000000000	۲۲ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶ ۲۶	0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.0000000E+00 0.000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.00000E+00 0.000000E+00 0.00000E+00 0.000000E+00 0.000000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+	TABLE OF CONCENTRA           Perster of concentra           Perster of concentra           Solution persmec           Solution           Solution     <
			≫4[0 <b>X</b> [€10]	<pre>\J CJPSIGE EFGCLIOU EFGCLIOU EFGCLIOU BUDCAC CIO4-(ET) MD(A) MD(A) Ym(III) Ym(II)</pre>	000000000E+000 # 1383111842 & d 3-,7 	EX cλ 0.000000 out 1188.00 sout 1188.00 eq peuzicλ fiserc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc drawc	0.000000000000000000000000000000000000	LPBTE OL CONCENLEY belgent rejeting Dewith paramer 2017110N AOF 2017110N AOF 2017110N AOF 1D2 AV72 1D2 AV72 2017110N AV72 2017110N AV72 2017110N AV72 100000000E+00 0.00000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.000000E+00 0.00000E+00 0.000000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.00000E+00 0.00000E+00 0.000000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.000
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				<ul> <li>J</li> <li>CIPSTGE</li> <li>EJECCIOU</li> <li>EJECCIOU</li> <li>BLOOEDDUTR</li> <li>CIOC-(ET)</li> <li>MD(A)</li> <li>MD(A)</li> <li>MD(A)</li> <li>MITIN</li> <li>MULTIN</li> <li>MOLOU</li> <li>MOLOU</li></ul>	<pre>000+300000000 \$</pre>	ελ         0.0000000           ελ         0.000000           ους         1788.60           ους         1788.60           ους         1788.60           ες         0.000000           ες         0.000000           ες         1788.60           ες         1788.60           ες         ες	0.000000025-00 0 0.00000025-00 0 0.00000025-00 0 0.00000025-00 0 0.00000025-00 0 0.000000025-00 0 0.0000000025-00 0 0.000000025-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.00000005-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.00000005-00 0 0.000000005-00 0 0.000000005-00 0 0.000000005-00 0 0.00000000000 0.0000000000 0 0.0000000000	LPBTE OL CONCENLEY Deuzità pereq ou percent rejettae 2014100 ADT 2014100 Extemen 2014100 Extemen 2014100 Extemen 2014100 Extemen 2014100 Externe 2014100 Externe 2014100 Externe 2014100 Externe 2014200000000 0 000000000000 0 00000000000
				<pre>\J CJPTLGe CJPTLGe EJectiou EJectiou EJectiou Dicto-(ET) Dicto-(ET) Dictin Dictin Dictin Dictin Colociuu Necliou Necliou</pre>	<pre>00000000E+000 # 000000E+000 # 0000000E+00 0000000E+00 0000000E+00 0000000E+00 0000000E+00 00000000</pre>	EX εX εX εX εX εX εX εX εX εX ε	<pre>2.4101 4325E+00 5 2.41030000E+00 0 2.41030000E+00 0 2.410300000E+00 0 2.445491025424 2.410347792 2.451025424 2.12485491025425 2.4103477592 2.451025424 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.1248549125425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.12485491025425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255425 2.124854910255455 2.124854910255455 2.124854910255455 2.1248545455555555555555555555555555555555</pre>	LPPTE OF CONCENTRA percent relative Density based on persity based on Solution Persmet Solution Persmet Solution Persmet Solution Persmet Persective Solution (0,0000005+00 -1,85232941E-15 Solution Persmet Solution Persmet -1,85232941E-15 -1,85232941E-15 -1,85232941E-15 -1,95232941E-15 -1,95232941E-15 -1,95232941E-15 -1,95232941E-15 -1,95232941E-15 -1,95232941E-15 -1,95232941E-15 -1,95232941E-15 -1,9523941E-15 -1,9523941E-15 -1,9523941E-15 -1,9523941E-15 -1,952492400 -1,954984805+00 -1,964984805+00 -1,964984805+00 -1,00000005+00 -1,00000005+00 -1,95498405+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,0000005+00 -1,0000005+00 -1,0000005+00 -1,0000005+00 -1,000005+00 -1,0000005+00 -1,0000005+00 -1,0000005+00 -1,0000005+00 -1,0000005+00 -1,0000005+00 -1,0000005+00 -1,00000005+00 -1,00000005+00 -1,0000005+00 -1,0000005+00 -1,00000005+00 -1,00000005+00 -1,0000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,0000005+00 -1,00000005+00 -1,0000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,0000005+00 -1,0000005+00 -1,0000005+00 -1,00000005+00 -1,0000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,00000005+00 -1,000000000000000000000000000000000000
				/] CDATGE Election Election Clot-(EL) Magnesium Magnesium Magnesium Solin Alist Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Solin Sol	<pre>3000000000000000000000000000000000000</pre>	ελ         0.0000000           ελ         0.000000           ους         1788.60           ους         1788.60           ους         1788.60           ες         0.000000           ες         0.000000           ες         1788.60           ες         1788.60           ες         ες	<pre>4 25 56624986E+01 4</pre>	LPBTE OL CONCENLEY BELCENE LEJFETAG DENETEA CONCENLEY DENETEA CONCENLEY 201701000000000000000000000000000000000

Appendix P: Sample Output File "Np_NaCl_BM.OUT"

FMT, Version 2.0 User's Manual, Version 1.00 · .....

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Appendix P: Sample Output File "Np_NaCl_BM.OUT"

MOLES file name is U1: (SCBABB.FMT.USERGUIDE)NP_NACL_BM.MOLES; 1



-. Appendix Q: Sample Output File "BATCH_DOC.FOR088"

## Appendix Q: Sample Output File "BATCH_DOC.FOR088"

## See Table 28 for explanation of this listing.

		1.11 filmen	5.550868155779565E+01
	5.506118174079332E+01		••••
i'r			2.016254639034410E-01
*			1.008127319517206E-02
4	9.930829876074504E-05		1.001154090354837E-04
-	1.089876985084734E+08		1.098734763576966E-08
U	3.514119485249377E-08		3.5426798571276352-08
	1.916539289681380E-13	H+ H+	1.932115616855898E-13
εk.	1.099999999999999998-01	C1- C1-	1.108940051468925E-01
4	9.9999999999959653E-04		1.008127319513137E-03
د :	4.0351912409451922-15	HS04- HS04-	4.067986529473380E-15
11	9.800006626741904E-02		9.879654411868162E-02
12	1.092064419243065E+07		1.100939975711625E-07
	9.9199126039D5744E-05		1.000053490322044E-04
٢.	2.193596324554590E-14		2.211424382786093E-14
10	6.916147055733898E-07		6.972356792683824E-07
	5.279149790754905E-11		5.322055127883555E-11
	1.640770852300863E-11		1.654105921272029E-11
	9.989705247502765E-08		1.0070894773931922-07
	0.000000000000000000E+00		0.0000000000000000E+00
2	0.00000000000000000E+00	B405 (0H) 4= B405 (0H) 4=	0.00000000000000E+00
			8.723697139181022E-11
2	6.134836150886349E~15	MoB (OH) 4+ MoB (OH) 4+	6.184695924470303E-15
	0.00000000000000000E+00	Br- Br-	
	0.000000000000000000000000000000000000		0.0000000000000000000000000000000000000
20		NaOH(aq)to.titrate.base.only	0.0000000000000000000000000000000000000
20		HCl(aq)to.titrate.acid.only	
27		HC104(aq)to.titrate.acid.only	
		PoslonPOSITIVE.ION	
		NeglonNEGATIVE.ION	
		PosIon(OH) (aq) to.titrate.base	
21		HNegIon(aq)to.titrate.acid	
2.2	0.0000000000000000E+00	Tracer(aq)conservative.tracer	0.00000000000000E+00
3.3	0.00000000000000000000E+00	H3P04 (ag) H3P04 (ag)	0.00000000000000E+00
1.2	0.00000000000000000E+00	H2P04 - H2P04 -	0.00000000000000000±+00
	0.0000000000000000E+00		0.0000000000000002+00
30	0.000000000000000E+00	P04=- P04=-	0.00000000000000E+00
27	0.00000000000000000E+00	NpO2+ NpO2+	0.00000000000000000E+00
22	0.0000000000000000E+00	NpO2OH(aq) NpO2OH(aq)	0.000000000000000000000000000000000000
	0.000000000000000000E+00		0.0000000000000000E+00
4.5			0.000000000000000E+00
11	0.00000000000000000E+00		0.000000000000000000000000000000000000
42	0.00000000000000000E+00	Np02 (C03) 3==- Np02 (C03) 3==-	0.000000000000000E+00
~3	0.00000000000000000E+00	Am+++ Am+++	0.0000000000000000E+00
-			0.0000000000000000000000000000000000000
			0.0000000000000000000000000000000000000
10	0.000000000000000000000000000000000000	Am(CO3)3=- Am(CO3)3=-	0.000000000000000E+00
12	0.0000000000000000000E+00		
		Am (OH) 2+ Am (OH) 2+	
15	0.00000000000000002+00	Am (OH) 2+ Am (OH) 2+ Am (OH) 3 (arr)	0.00000000000000E+00
43	0.0000000000000000E+00	Am(OH)3(ag) Am(OH)3(ag)	0.000000000000000000000000000000000000
~	0.00000000000000000E+00 0.00000000000000	Am(OH)3(ag)         Am(OH)3(ag)           Th++++         Th++++	0.000000000000000000000000000000000000
~	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           102++         11(VI) 02++	0.000000000000000000000000000000000000
~	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           102++         11(VI) 02++	0.000000000000000000000000000000000000
~	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           102++         11(VI) 02++	0.000000000000000000000000000000000000
	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           UO2++         U(VI) 02++           Np02OH (aged)         Np02OH (aged)           Np02OH (amor)         Np02OH (aged)           NaNp02CO3 (s)         NaNp02CO3 (s)	0.000000000000000000000000000000000000
	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           V02++         U(V1)02++           Np02OH (aged)         Np02OH (aged)           Np02OH (amor)         Np02OH (amor)           NaNp02C03 (s)         NaNp02C03 (s)           NaNp02C (C03) 2 (s)_DISABLED_DISABLED         DISABLED_DISABLED	0.000000000000000000000000000000000000
	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           U02++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           Np02OH (agod)         Np02OH (aged)           Np02OH (agod)         Np02OH (agod)           NaNp02C03 (s)         NaNp02C03 (s)           NaNp02C03 (c)         AmOHC03 (c)           Am(OH3 (c)         AmOHC03 (c)	0.000000000000000000000000000000000000
	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           U02++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           Np02OH (agod)         Np02OH (aged)           Np02OH (agod)         Np02OH (agod)           NaNp02C03 (s)         NaNp02C03 (s)           NaNp02C03 (c)         AmOHC03 (c)           Am(OH3 (c)         AmOHC03 (c)	0.000000000000000000000000000000000000
	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           U02++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           Np02OH (agod)         Np02OH (aged)           Np02OH (agod)         Np02OH (agod)           NaNp02C03 (s)         NaNp02C03 (s)           NaNp02C03 (c)         AmOHC03 (c)           Am(OH3 (c)         AmOHC03 (c)	0.000000000000000000000000000000000000
	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           U02++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           Np02OH (agod)         Np02OH (aged)           Np02OH (agod)         Np02OH (agod)           NaNp02C03 (s)         NaNp02C03 (s)           NaNp02C03 (c)         AmOHC03 (c)           Am(OH3 (c)         AmOHC03 (c)	0.000000000000000000000000000000000000
	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           UO2++         U(VI) 02++           MpO2OH (aged)         MpO2OH (aged)           MpO2OH (amor)         NpO2OH (amor)           NaNpO2CO3 (s)         NaNpO2O3 (s)           Ma3NpO2 (CO3) 2 (s)         DISABLED           AmOHCO3 (c)         AmOHCO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaMPO4 (c)         AmPO4 (c)	0.000000000000000000000000000000000000
**************************************	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           UO2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (agod)         NpO2OH (agod)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           AmOHCO3 (c)         NaNPO2CO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaAm(CO3) 2.6H2O (c)         AmPO4 (c)           CaSO4         Anhydrite           NaX1 (SO412         Aphthitalite/Glaserite	0.000000000000000000000000000000000000
* 20 8 5 8 8 5 8 8 5 0 F	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (aged)         NpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNPO2CO3 (c)         AmOHCO3 (c)           AmOHCO3 (c)         AmOHCO3 (c)           AmOHCO3 (2) 2.6H2O (c)         AmOHCO3 (c)           AmPO4 (c)         AmPO4 (c)           CaS04         Anhydrite           NaX3 (SO4) 2_Aphthitalite/Glascrite         Cal2.6H2O	0.000000000000000000000000000000000000
そうじゅう かいかい ひょうしん	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (aged)         NpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           AmOHCO3 (c)         NanOHCO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaAm(CO3) 2. 6H2O (c)         AmPO4 (c)           CaSO4         Anhydrite           NaX3 (SO4) 2_Aphthitalite/Glaserite         CaCO3           CacO3         Aragonite	0.000000000000000000000000000000000000
そうじゅう かいかい ひょうしん	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (aged)         NpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           AmOHCO3 (c)         NanOHCO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaAm(CO3) 2. 6H2O (c)         AmPO4 (c)           CaSO4         Anhydrite           NaX3 (SO4) 2_Aphthitalite/Glaserite         CaCO3           CacO3         Aragonite	0.000000000000000000000000000000000000
そうじゅう かいかい ひょうしん	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (aged)         NpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           AmOHCO3 (c)         NanOHCO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaAm(CO3) 2. 6H2O (c)         AmPO4 (c)           CaSO4         Anhydrite           NaX3 (SO4) 2_Aphthitalite/Glaserite         CaCO3           CacO3         Aragonite	0.000000000000000000000000000000000000
そこうほうそうとう ほうくりゅう かん	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (aged)         NpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           AmOHCO3 (c)         AmOHCO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaAm(CO3) 2. 6H2O (c)         Am(OH) 3 (s)           AmOHCO3 (c)         AntoHvG1 (c)           CaSO4         Anthvdrite           NaX3 (SO4) 2_Aphthitalite/Glaserite         CaCO3           CaC03         Artagonite           K2SO4         Artagonite           NaZMG (SO4) 2_6H2O         Bloedlite	0.000000000000000000000000000000000000
そこうほうそうとう ほうくりゅう かん	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (aged)         NpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           AmOHCO3 (c)         AmOHCO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaAm(CO3) 2. 6H2O (c)         Am(OH) 3 (s)           AmOHCO3 (c)         AntoHvG1 (c)           CaSO4         Anthvdrite           NaX3 (SO4) 2_Aphthitalite/Glaserite         CaCO3           CaC03         Artagonite           K2SO4         Artagonite           NaZMG (SO4) 2_6H2O         Bloedlite	0.000000000000000000000000000000000000
そこうほうそうとう ほうくりゅう かん	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (aged)         NpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           AmOHCO3 (c)         AmOHCO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaAm(CO3) 2. 6H2O (c)         Am(OH) 3 (s)           AmOHCO3 (c)         AntoHvG1 (c)           CaSO4         Anthvdrite           NaX3 (SO4) 2_Aphthitalite/Glaserite         CaCO3           CaC03         Artagonite           K2SO4         Artagonite           NaZMG (SO4) 2_6H2O         Bloedlite	0.000000000000000000000000000000000000
そこうほうそうとう ほうくりゅう かん	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH (aged)         NpO2OH (aged)           NpO2OH (aged)         NpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           AmOHCO3 (c)         AmOHCO3 (c)           Am(OH) 3 (s)         Am(OH) 3 (s)           NaAm(CO3) 2. 6H2O (c)         Am(OH) 3 (s)           AmOHCO3 (c)         AntoHvG1 (c)           CaSO4         Anthvdrite           NaX3 (SO4) 2_Aphthitalite/Glaserite         CaCO3           CaC03         Artagonite           K2SO4         Artagonite           NaZMG (SO4) 2_6H2O         Bloedlite	0.000000000000000000000000000000000000
そこうとなるというななりをあるとのででの	0.000000000000000000000000000000000000	Am(OH)3(aq)         Am(OH)3(aq)           Th++++         Th++++           VD2++         U(V1)02++           NpO2OH(aged)         NpO2OH(aged)           NpO2OH(amor)         NpO2OH(amor)           NaNpO2CO3(s)         NaNpO2CO3(s)           Am(OH)3(aq)         NpO2OH(amor)           NaNpO2CO3(s)         NaNpO2CO3(s)           AmOHCO3(c)         AmOHCO3(c)           Am(OH)3(s)         Am(OH)3(s)           NaAm(CO3)2.6H2O(c)         AmCOH(O)3(s)           AmOHCO3(c)         AmOHCO3(c)           Am(OH)3(s)         AmOHCO3(c)           AmOHCO3(c)         AmOH(O)3(s)           NaX3(SO412_Aphthitalite(Glaserite         CaC03_Aragonite           K2S04         Arcanite           Mg(OH)2Blocdite         Blocdite           Mg(OH)2Brucite         RaC03 (SO4)2_Burkeite           CaC03CaCl2_Cacl2_Tetrahydrite         Cacl2	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           VD2++         U(V1)02++           Np02OH (aged)         Mp02OH (aged)           NaNp02C03 (s)         NaNp02C03 (c)           Am(OH) 3 (s)         NaAm (OH) 3 (s)           NaAm (CO3) 2.6H2O (c)         Am OH(3 (s)           AmBO4 (c)         CaS04 (aged)           Antaroticite         CaC12.6H2O (c)           Antaroticite         CaC12.6H2O (c)           MaxX (SO4) 2         Aphthitalite /claserite           MgC12 6H2O (c)         Bischofite           Mg(OH) 2         Bischofite           MaCO3 (SO4) 2         Burkeite           CaC12 (SO4) 2         Calcite           CaC12 (AH2O)         Calcite           CaC12 (CH 6.13H2O_CaOxychloride A	0.000000000000000000000000000000000000
*2.113.234.2227.354.04.024.44.004.207.202.	0.000000000000000000000000000000000000	Am (OH) 3 (aq)         Am (OH) 3 (aq)           Th++++         Th++++           UO2++         U(V1)O2++           NpO2OH (aged)         MpO2OH (aged)           NpO2OH (aged)         MpO2OH (aged)           NaNpO2CO3 (s)         NaNpO2CO3 (s)           NaNpO2CO3 (c)         AmOHCO3 (c)           Am(OH) 3 (s)         AmOHCO3 (c)           AmOHCO3 (c)         AmOHCO3 (c)           AmOHCO3 (c)         AmOHCO3 (c)           AmOHCO3 (c)         AmOHCO3 (c)           AmBO4 (c)         AmOHCO3 (c)           AmBO4 (c)         AmOHCO3 (c)           AmOHCO3 (c)         AmOHCO3 (c)           AmOHCO3 (c)         AmOHCO3 (c)           Mam (OCO3) 2. 6H2O (c)         AmOHCO3 (c)           AmBO4 (c)         CaSO4           Antarcticite         CaCl2.6H2O           CaCl2 (H2O         Bischoffite           Mg (OH) 2         Birceite           MaCO3 (SO4) 2         Birceite           CaCO3         Calcite           CaCO3         Calcite           CaCO3         Calcite           CaCl2 (OH) 6.13H2O         Calcite/Lorde	0.000000000000000000000000000000000000



# Appendix Q: Sample Output File "BATCH_DOC.FOR088"

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23	0.0000000000000000000000000000000000000	Na4Ca(SO4)3.2H20Labile_Salt	0 0000000000000000000000000000000000000
4.1		MgC03Magnesite	
÷		Mg2Cl(OH)3.4H20Mg0xychloride	
		KHS04Mercallite	
27	B_000000000000000000000000000000000000	Na2SO4.10H20Mirabilite	0 0000000000000000000000000000000000000
25		K8H6 (504) 7Misenite	
85		NaHCO3Nahcolite	
- ží			
5 E	0 0000000000000000000000000000000000000	Na2CO3.10H20Natron MgCO3.3H20Nesquehonite	0.00000000000000000E+00
52	0 0000000000000000000000000000000000000	K2Mg(SO4)2.6H2O Picromerite/Schoen	0.0000000000000000E+00
		Na2Ca(CO3)2.2H2OPirssonite	
34.	0.0000000000000000000000000000000000000	K2McCa2(SO4)4.2H20 Polyhalite	0.000000000000000E+00
2.1	0.000000000000000E+00	Ca(OH)2Portlandite	0,00000000000000000E+00
25	0.000000000000000E+00	K2CO3.3/2H20 Potassium_Carbonate	0.0000000000000000E+00
4		K8H4(CO3)6.3H20K-Sequicarbonate	
	0.000000000000000E+00	KNaCO3.6H20K-Na-Carbonate	0.0000000000000000E+00
	0.000000000000000E+00	K2NaH(CO3)2.2H20Potassium_Trona	0.0000000000000000E+00
100	0.00000000000000E+00	K3H(SO4)2Sesquipotassium_Sulfate	0.000000000000000E+00
100	0.000000000000000E+00	Na3H(SO4)2Sesquisodium_Sulfate	0.0000000000000000E+00
<b>*</b> .1		Na2CO3.7H2ONa2CO3-Heptahydrate	
. U .	0.00000000000000E+00	KClSylvite	0.000000000000000E+00
104		K2Ca(SO4)2.H20Syngenite	
100		Mg2CaCl6.12H20Tachyhydrite	
<u>,</u>		Na2SO4Thenardite	
· . : 7		Na2CO3.H20Thermonatrite	
\$5	0.0000000000000000E+00	Na3H(CO3)2.2H20Trona	0.000000000000000000000000000000000000
. Oc	0.0000000000000000E+00	Na2B407.10H20Borax B(OH)3Borix_Acid_Solid	0.000000000000000E+00
: * :	0.0000000000000000E+00	B(OH) 3Borix_Acid_Solid	0.000000000000000±+00
•••		KB508.4H20K-Pentaborate_(30_C)	
		K2B407.4H20K-Tetraborate_(30_C)	
		NaBO2.4H20Sodium_Metaborate	
		NaB508.5H20Sodium_Pentaborate	
1.5	0.0000000000000000E+00	NaBO2.NaCl.2H20Teepleite_(20_C)	0.00000000000000000E+00



Appendix R: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

## Appendix R: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

29 for explanation of this listing.

		L.31 Am(III)	-Na-C1-C03-S04			.,	,				
	Titre	unt Volumes pe	r Grid Block,	in milliliters							
0	1		000000 mL								
•	2		100000 mL								
Т. Ц	3		142510 mL								
	4		203092 mL 289427 mL							05 m	A. May
• · ·	6		412463 mL							and the state of t	
- 2	7		587802 mL							¢ ·	
t?	8		837678 mL							ŝ	1
1	9		193777 mL							tan an a	•
•	10 11		701254 mL 424462 mL								
- ?	12		455107 mL							ka in	• •
2	13		923883 mL							*****	
14	14		017038 mL							·~~	140 V 214 V
20	15	10.	000000 mL								
3	Titra	tion Results,	molal								
		н20	Na+	K+	Ca++	Mg++	MgOH+	H+	C1-	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	5.61014£+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.77346E-07	5.60993E+00	0.00000E+00	
4. -	3)	1.929998+01	5.61003E+00 5.61000E+00	0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	2.58813E-07	5.60950E+00	0.00000E+00	
	4) 5)	1.93029E+01 1.93072E+01	5.61000E+00	0.00000E+00 0.00000E+00	0.0000DE+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	2.91065E-09 3.42512E-10	5.60889E+00 5.60800E+00	0.00000£+00 0.00000£+00	
2	6)	1.93133E+01	5.61000E+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	1.52979E-10	5.60673E+00	0.00000E+00	
22	7)	1.93221E+01	5.61001E+00	0.00000E+00	0.0000E+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	0.0000E+00	0.00000E+00	0.00000E+00	5.44489E-11	5.60233E+00	0.00000E+00	
5	9)	1.93524E+01	5.61002E+00 5.61003E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.62550E-11	5.59866E+00	0.00000E+00	
.;	10) 11)	1.93778E+01 1.94140E+01	5.61003E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	2.51081E-11 1.79163E-11	5.59343E+00 5.58601E+00	0.00000E+00	
3	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 0.00000E+00	
30	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	
12	14)	1.964372+01	5.61021E+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	7.48733E-12	5.53952E+00	0.0000E+00	
	15)	1.97930E+01	5.61035E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	5.83272E-12	5.50989E+00	0.00000E+00	
2 :0		HS04-	OH-	HC03-	CO3=	CO2 ( ad)	(20)	Naccol (and)	D (011) 2 ()	D ( 011) 4	
	1)	0.00000E+00	3.01685E-09	2.26571E-04	3.09384E-08	CO2(aq) 3.86103E-04	CaCO3 (aq) 0.00000E+00	MgCO3 (aq) 0.00000E+00	B(OH)3(aq) 0.00000E+00	B(OH)4- 0.00000E+00	
13	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	
5	3)	0.00000±+00	1.42123E-08	5.79856E-04	3.72979±-07	2.09763E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
0	4)	0.00000E+00	1.26397E-06	9.92660E-04	5.67888£-05	4.03745E-06	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
ः .२	5) 4)	0.00000E+00 0.00000E+00	1.07447E-05 2.40584E-05	1.00903E-03	4.90717E-04 1.11398E-03	4.82702E-07	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00	
	6) 7)	0.00000E+00	4.24988E-05	1.02256E-03 1.04073E-03	2.00201E-03	2.18328E-07 1.25799E-07	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	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)	0.0000E+00	1.01865E-04	1.09867E-03	5.06627E-03	5.53405E-08	0.00000E+00	0.00000E+00	C.00000E+00	0.00000E+00	
3	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	
<i>!</i>	11)	0.00000E+00	2.07123E-04	1.20082E-03	1.12609E-02	2.96765£-08	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
a	12) 13)	0.00000±+00 0.00000±+00	2.84255E-04 3.82200E-04	1.27533E-03 1.36956E-03	1.64154E-02 2.37058E-02	2.29199E-08 1.82542E-08	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
7	14)	0.00000E+00	5.04619E-04	1.48672E-03	3.39812E-02	1.49488E-08	0.00000£+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	C.COCOOE+00 C.COCOOE+00	
5 5 -	15)	0.0000E+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-	B405 (0H) 4≠	CaB (OH) 4+	MgB (OH) 4+	Br-	C104-	NaOH (ag)	HC1 (ag)	HC104 (ag)	
	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	2)	0.00000£+00	0.00000£+00	0.00000E+00	0.0000E+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	0.00000000000	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
	4) 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 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
с С	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 0.00000E+00	0.00000E+00 0.00000E+00	
;	7)	0.00000E+00	0.00000E+00	0.000002+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	0.0000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
2	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	
	10) 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 0.00000E+00	0.00000E+00 0.00000E+00	C.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	0.000005+00	0.00000E+00	0.00000E+00	0.00000E+00	
	14)	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
>	15)	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.000002+00	0.00000E+00	
2		Posion	NegTon	Postor (OV) (	HNegles(ta)	Tracer()	H3B04 ()	¥2004	ND04-	<b>0</b> 04-	
		0.00000E+00	NegIon 0.00000E+00	0.00000E+00	(HNegIon(ag) 0.00000E+00	Tracer(aq) 0.00000E+00	H3PO4 (aq) 0.00000E+00	H2PO4~ 0.00000E+00	HF04= 0.00000E+00	PO4=- 0.00000E+00	
5	T.)									0.00000E+00	
	1) 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	
	2) 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	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	
	2)	0.00000E+00									

.. .

# Appendix R: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	C.00000E+00	0.00000£+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	
4. C	B)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
÷C.	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	
21	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	
ĉć	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	
27	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	
2.2	13}	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
÷.	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000CE+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
52	15)	0.00000E+00	0.00000E+00	0.00000£+00	0.00000£+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
۰.											
100		Np02+	NpO20H(aq)	NpO2 (OH) 2-	Np02C03-	Np02 (C03) 2×-	NpO2 (CO3)3==-		AmCO3+	Am (CO3)2-	
02 13	1)	5.12705E-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	
53	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)	5.08519E-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	
×2	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	
1.1	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	0.0000E+00	0.0000E+00	
.'	7)	9.49498E-09	1.68316E-10	6.28105£-13	1.33688E-07	1.28137E-06	5.19502E-07	0.00000E+00	0.0000E+00	0.00000E+00	
· · ·	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	
<u></u>	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	1.535838-10	1.99131E-12	1.33905E-07	4.85191E-06	7.39875E-06	0.00000E+00	0.0000000+00	0.00000E+00	
÷CC	11)	1.70329E-09	1.46370E-10	2.67040E-12	1.34044E-07	7.13717E-06 1.03463E-05	1.59398E-05 3.32873E-05	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	
3	12)	1.17432E-09	1.38078E-10	3.46327E-12 4.35852E-12	1.34242E-07 1.34522E-07	1.48219E-05	6.77047E-05	0.00000E+00	0.00000E+00	0.00000E+00 0.00000E+00	
ية. طي خ	13) 14)	8.18986E-10 5.77122E-10	1.28920E-10 1.19205E-10	4.35852E-12 5.33952E-12	1.34916E-07	2.10028E-05	1.34208E-04	0.00000E+00	0.00000E+00	0.00000E+00	
يەن :	14)	4.11022E-10	1.09291E-10	6.38945E-12	1.354681-07	2.94209E-05	2.58546E-04	0.00000E+00	0.00000E+00	0.00000E+00	
	1 - 1		1								
		Am (CO3) 3=-	Am (OH) 2+	Am (OH) 3 (aq)	Th++++	UO2++	NpO20H(aged)	NpO2OH(amor)	NaNp02C03(s)	Na3Np02(C03)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	
1.1	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.000006+00	0.00000E+00	0.000002+00	0.00000£+00	9.99473E+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	9.99250E+00	0.00000E+00	
••,	6)	0.00000E+00	0.00000E+00	0.00000£+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	9.98931E+00	0.0000E+00	
512	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98478E+D0	0.00000E+00	
- 13	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	
12-	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00	0.000002+00	9.95607E+00	0.0000002+00	
122	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.93751E+00	0.0000DE+00	
	12)	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.91117E+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	9.87386E+00 9.82115E+00	0.00000E+00	
25	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.000002+00	9.74696E+00	0.00000E+00 0.00000E+00	
	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.000002+00	0.00000E+00	0.000002+00	9./N090E+UU	0.00005+00	
11.2 102		AmOHCO3 (c)	2-(01)7(0)	_ NaAm (CO3) 2.6H		CaS04	NaK3 (SO4) 2A	CaC12 6820	CaC03	K2504	
	11		_ Am (OH) 3 (s) 0.00000 E+00				0.00000E+00				
123	1)	0.000002+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00 0.00000E+00		0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	
123	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	
	2) 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 0.00000E+00	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 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	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) 3) 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 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	
※第二、二、二、二、二、二、二、二、二、二、二、二、二、二、二、二、二、二、二、	2) 3) 4) 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 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	
꼜흕똜뜺슻 _녇 읁敛	2) 3) 4) 5) 6)	0.000002+00 0.000002+00 0.000002+00 0.000002+00 0.000002+00 0.000002+00 0.000002+00 0.000002+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.000000000000000000000000000000000000	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	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) 3) 4) 5) 6) 7) 8) 9)	0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00 0.00002+00	0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	0.0000E+00 0.0000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	
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Appendix R: Sample Output File "Np_NaCl_BM_LOG.TITRATE"

:73	11)	0,000002+00	0.D0000E+00	0.000005+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+D0	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	0.00000£+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
.70	14)	0.0000000+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
177	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	0.00000£+00	0.00000E+00	0.00000E+00
	751	0.000002+00				•				
- 73		K2Ma (SO4) 2,4H	Na4Ca(SO4)3.2	MgCO3	Mg2C1(OH)3.4H	KHSQ4	Na2S04.10H20_	K8H6 (SO4)7	NaHCO3	Na2CO3.10H20_
ريم ۲	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	Q.00000E+00	0.00000E+00
	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00
		0,00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000£+00	0.00000E+00	0.00000E+00
	3)		0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	D.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
150	4)	0.000002+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
۶۰.	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
	7)	0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
502 1	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
122	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
3	10)	0.00000E+00	0.00000E+00		0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00
20	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			
<b>.</b>	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	D.00000E+00	0.00000E+00	0.00000E+00
163	14}	0.00000E+00	0.00000E+00	0.00000£+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
194	15)	0.00000E+00	0.00000£+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.0000E+00
100										1731-11/00330 D
<b>`</b>		MgCO3.3H20			K2MgCa2(SO4)4			K8H4 (CO3) 6.3H		
97	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	0.0000E+00
195	2)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
199	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
201	4}	0.00000E+00	0.00000E+00	D.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00
201	5}	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.0000E+00	0.00000E+00	0.000000000000	0.00000E+00
$\langle \cdot \cdot \rangle$	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000£+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000£+00	0.00000E+00
10	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	8)	0.000005+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000£+00
20	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	0.0000E+00
XX.	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00
007	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.0000E+00	0.0000E+00
150	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00
2-33	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	D.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
∠*-2	14)	0.00000E+00	0.00000E+00	0.00000£+00	0.00000E+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.0000E+00
211	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.12										
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		K3H(S04)2Se	Na3H(SO4) Z	Na2C03.7H20	KC1	K2Ca(SO4)2.H2	Mg2CaCl6.12H2	Na2SO4	Na2CO3.H2O	Na3H(CO3)2.2H
17.	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	0.00000£+00
21.5	2)	0,00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000±+00	0.00000E+00	0.00000E+00
210	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
317	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00002+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	0.000002+00	0.00000E+00	0.0000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
22.7	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	D.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00
221	81	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	D.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
322	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000£+00	0.00000E+00
273	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
224	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
225	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00
. 2:	13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
227	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	0.00000E+00
2.5	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
226										
		Na2B407.10H20	B(OH)3	KB508.4H20	K2B407.4H20	NaBO2 . 4H2O	NaBS08.5H20	NaBO2.NaC1.2H		
231	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
233	2	0.00000E+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
233	3)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
2.4	4)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
205	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
236	6)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		
237	7)	0.00000E+00	0.00000E+00	0.00000E+00	0.0000000+00	0.00000E+00	0.00000E+00	0.00000E+00		
2:32	8)	0.00000E+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		·
233	9)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		N.
2.00	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00		
24	11)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	<u>:</u>	 ≤ 1 ≤ 1
12	12)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		10 NO 1
212	131	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	C.00000E+00	0.000005+00	0.00000E+00	1 No. 4	Seine State
262	14)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1 10	Stell 1
245	15)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		6. × /
24-5	*21	0.000002.00		0.000002.00	0.00002.00	0.000000.00	0.000002+00	0.000000+00		No. /
247		IonicStreng	Eh{=}Volts	TitrVol,ml	pH					
243	1)	5.61119E+00	0.00000E+00	0.000002+0						
243	2)	5.61031E+00	0.00000E+00	0.10000	5.6451					
250	3)	5.61008E+00	0.00000E+00	0.14251	5.9936					
251	4}	5.61008E+00	0.00000E+00	0.20309	7.9427					
250	5)	5.61049E+00	0.00000E+00	0.28943	8.8722					
203										
264	6) 7)	5.61112E+00 5.61202E+00	0.00000E+00 0.00000E+00	0.41246 0.58780	9.2225 9.4695					
285	8)	5.61202E+00 5.61330E+00	0.000000000000	0.83768	9,4695					
252										
250	9)	5.61513E+00	0.00000E+00	1,1938	9.8493					
	10)	5.61774E+00	0.00000000000	1.7013	10.010					
8-5. 936.	12)	5.62149E+00	0.00000E+00	2.4245	10.158					
000	12}	5.62685E+00	0.00000E+00	3.4551	10.295					
	13)	5.63455E+00	0.00000E+00	4.9239	10.424					
201	14)	5.64559E+00	0.000002+00	7.0170	10.545					
262	15)	5.66143E+00	0.00000E+00	10.000	10.659					



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5.61096E+00

5.60993E+00

5.60685E+00

5.60479E+00

5.60375E+00

5,60066E+00

5.59859E+00

5.59756E+00

5.59653E+00

B(OH)3(ag)

0.00000E+00

0.000005+00

0.00000E+00

00000E+00

00000E+00

00000E+00

60892E+00

60789E+00

60582E+00

60272E+00

60169E+00

59962E+00

1.21872E-06

5.77346E-07

3.87609E-09

3.09202E-10

1.61951E-10

1.10445E-10

8.42049E-11

6.82959E-11

5.76161E-11

4.99485E-11

4.41741E-11

3.96673E-11

3.30838E-11

3.06048E-11

0.00000E+00

0.00000E+00

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MgCO3 (ag)

60509E-11

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SO4 =

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0.00000E+00

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B(OH)4-

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MgOH+

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CaCO3 (ag)

00000E+00

00000E+00

00000E+00

Appendix S: Sample Output File "Np_NaCl_BM_LIN.TITRATE"

Appendix S: Sample Output File "Np_NaCl_BM_LIN.TITRATE"

Ca++

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.000002+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.000002+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

3.09364E-08

1.10196E-07

4.25167E-05

5.44263E-04

1.05085E-03

1.55739E-03

2.06377E-03

2.56997E-03

3.07597E-03

4 08730E-03

4.59262E-03

5.602538-03

6.10711E-03

.09770E-03

.58175E-03

CO3=

0.00000E+00

0.00000E+00

0.00000E+00

0.000002+00

0.000002+00

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0.000002+00

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2.26571E-04

3.82212E-04

9.89705E-04

1.01025E-03

1.02124E-03 1.03174E-03

1.04196E-03

1.05196E-03

1.06176E-03

1.07138E-03

1 08082E-03

1.09010E-03

1.09923E-03

1.10821E-03

1.11706E-03

HCO3-

Mg+4

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0

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3 5.36072E-06

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3.86103E-04

08476E-04

.36260E-07

.30850E-07

58957E-07

22321E-07

.00104E-07

44762E-08

50552E-08

8.51877E-08

6.64082E-08

6.01101E-08

5.09071E-08

4.74407E-08

CO2 (ag)

.00000E+00

.00000E+00

Benchmark TITRATE Problem, LINEAR option; Np(V)02 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

Na+

5.61057E+00

5.61014E+00

5,61000E+00

5.61000E+00

5.61000E+00

5.61000E+00

5.61001E+00

5.61001E+00

5.61001E+00

5,61001E+00

5.61002E+00

5 61002E+00

5.61002E+00

.61002E+00

61001E+00

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1	0.00000	ബ്
2	0.100000	an L
3	0.200000	mL.
4	0.300000	mL.
5	0.400000	mL
6	0.500000	nL.
7	0.600000	mL.
8	0.700000	mL
9	0.800000	mL.
10	0.900000	mL
11	1.000000	nL.
12	1.100000	ttL
13	1.200000	πL.
14	1.300000	mL.
15	1.400000	πL

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23 2.11

220232 22232

27 32 11)

33 13)

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57 57 58

50 81

Titration Results, molal

1.92928E+01

1.92978E+01

1.93027E+01

1.93077E+01

1.93127E+01

1.93177E+01

1.93227E+01

1.93277E+01

1.93327E+01

1.93377E+01

1.93427E+01

1.93477E+01

1.93527E+01

1.93577E+01

1.93627E+01

HS04-

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1)

2)

3) 4)

5)

6) 7)

8)

91

10)

12)

14)

151 1.2

9)

10) 11)

12)

13)

14)

15)

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	1004-	011-
1)	0.00000E+00	3.01685E-09
2)	0.000002+00	6.37029E-09
3)	0.00000E+00	9.49137E-07
4)	0.00000E+00	1.19027E-05
5)	0.00000E+00	2.27338E-05
6)	0.00000E+00	3.33488E-05
7)	0.00000£+00	4.37579E-05
8)	0.00000E+00	5.39719E-05

0.00000E+00

0.00000E+00

0.00000£+00

0.00000E+00

0.00000E+00

0.00000E+00

0.00000E+00

1.20768E-04 (missing species have zero amounts)

6.40010E-05

8

.38545E-05

.35411E-05

9.30687E-05

1.02445E-04

1.11676E-04

€ 1										
÷ 2		NpO2+	NpO2OH(ag)	NpO2 (OH) 2-	Np02C03-	Np02 (C03)2=-	Np02 (CO3) 3==-	Am+++	AmCO3+	Am (CO3) 2 -
2.3	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	0.0000E+00
64	2)	1.72085E-04	4.57851E-10	2.55903E-16	1.33573E-07	7.06677E-11	1.58546E-15	0.00000E+00	0.00000±+00	0.00000E+00
÷.,	3)	4,46247E-07	1.768652-10	1.47303E-14	1.33612E-07	2.72677E-08	2.35800E-10	0.00000E+00	0.00000E+00	0.00000E+00
CC	4)	3.48770E-08	1.73300E-10	1.81034E-13	1.33632E-07	3.46878E-07	3.85776E-08	0.00000E+00	0.000006+00	0.00000E+00
67	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
e e	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
63	7)	9.21138E-09	1.68120E-10	6.45975E-13	1.33690E-07	1.32081E-06	5.51937E-07	0.00000£+00	0.00000E+00	0.0000E+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
7.1	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
72	10)	5.31533E-09	1.635952-10	1.06147E-12	1.33749E-07	2.28868E-06	1.65423E-06	0.00000£+00	0.00000E+00	0.00000E+00
72	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	0.00000£+00	0.00000E+00	0.00000E+00
?>	13)	3.74015E-09	1.59537E-10	1.43661E-12	1.33807E-07	3.25216E-06	3.33 418E-0 6	0.00000E+00	0.00000£+00	0.00000E+00
Z 15	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
72	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	0.0000E+00
7.2										
1		Am (CO3)3=-	Am (OH) 2+	Am (OH) 3 (aq)	Th++++	U02++	NpC2OH(aged)_	NpO2OH(amor)_	NaNpO2CO3(s)_	Na3NpO2{CO3}2
20	1)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00	9.99932E+00	0.00000E+00
1	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	0.000002+00
81	3)	0.00000E+00	0.000002+00	0.00000E+00	0.0000DE+00	D.00000E+00	0.00000E+00	0.00000£+00	9.99481E+00	0.00000E+00
33	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
21	5)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00	0.00000£+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	0.00000£+00
18	7)	D.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"

87	8)	0.0000E+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	
35	91	0.00000E+00	0.00000E+00	0.00000E+00	0.00000£+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97930E+00	0.00000E+00	
59	101	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.97672E+00	0.00000£+00	
÷.;	111	0.00000E+00	0.00000£+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	
2.5	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	
50	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	
22	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	
6.7										0.00002.00	
\$-C		(missing spe	ecies have zer	o amounts)							
į. 7											
3:		IonicStreng	Eh[=]Volts	TitrVol,ml	pł	H					
00	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)	5.61004E+00	0.00000E+00	0.20000	7.8183						
102	4)	5.61055£+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						
11 TO	7)	5.61208E+00	0.00000E+00	0.60000	9.4821						
7 t. t. s.	8)	5.61259E+00	0.00000E+00	0.70000	9.5733						
10 r	9)	5.61310E+00	0.00000E+00	0.80000	9.6473						
106	10)	5.61362E+00	0.0000E+00	0.90000	9.7095						
10-1	11)	5.61413E+00	0.0000E+00	1.0000	9.7631						
110	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						
113	15)	5.61619E+00	0.00000E+00	1.4000	9.9232						





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Appendix T: Sample Output File "Np_NaCl_BM.TITRATE"

Appendix T: Sample Output File "Np_NaCl_BM.TITRATE"

Benchmark TITRATE Problem; Np(V)02 with CO3 in 5.61molal NaCl FMT V2.0 HMW84/FW86; Np(V)-Na-CO3-OH-C1-C1O4 (NR94); Ź DATABASE : Am(III)-Na-C1-C03-S04-P04 (FRSR89, FRF90, P91, RFFR92, RFF94, RRFF94) 95.01.31 Titrant Volumes per Grid Block, in milliliters 0 0 000000 mL 0.100000 mL 2 3 0.142510 mL ŗ 4 0 160000 mL 1) 1) 0.180000 mL 5 0.203090 mL 0 220000 mL 0.240000 mL 8 0.260000 mL Ş ٠, 10 0.289430 mL 0.412460 mL 11 0.587800 mL 12 13 1.193800 mL 3.455100 mL 14 15 10.000000 mL Titration Results, molal 21 25 24 H2Q Ca+-MgOH+ C1-SO4= 5.61057E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.000002+00 1.21872E-06 5.61096E+00 0.00000E+00 1.92928E+01 11 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 2) 5.61003E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 2.58815E-07 5.609508+00 0.00000E+00 3) 1.92999E+01 0.00000£+00 0.00000E+00 0.0000E+00 0.00000E+00 1.48381E-07 5.60933E+00 0.00000£+00 1 93007E+01 5.61001E+00 43 0.00000E+00 0.00000E+00 .00000E+00 5.60913E+00 5.61000E+00 0.00000E+00 Ó 5.09374E-08 ٥ .00000E+00 2 a 1.93017E+01 51 5.61000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 2.91107E-09 5.60889E+00 0.00000E+00 0000000 000000 1.93029E+01 0.00000E+00 0.00000E+00 5.608722+00 0.00000E+00 0.00000E+00 1.18855E-09 0.00000E+00 7) 1.93037E+01 5.61000E+00 .00000E+00 .00000E+00 5.60851E+00 1.93047E+01 5.61000E+00 D.00000E+00 0.00000E+00 Û ø 6.93877£-10 ۵ .00000E+00 8) 5.61000E+00 0.000002+00 0.00000E+00 0.00000E+00 0.00000E+00 4 89995E-10 5 608302+00 0 000008+00 9) 1.93057E+01 0.00000E+00 0.0000E+00 0.00000E+00 5.60800E+00 0.00000E+00 3.42501E-10 10) 1.93072E+01 5.61000E+00 0.000002+00 1.93133E+01 5.61000E+00 0.00000E+00 0.00000E+00 0 00000E+00 0 .00000£+00 .52981E-10 5.60673E+00 .00000E+00 \$ 11) 5.61001E+00 1.93221E+01 12) 0.000002+00 0 00000£+00 0.00000E+00 0.00000E+00 8.66958E+11 5.60491E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 5.59866E+00 0.00000E+00 3.62542E-11 2 13) 1.93524E+01 5.61002E+00 0.00000E+00 0.00000E+00 0.00000±+00 5.57548E+00 1.94655E+01 5.61007E+00 0.00000E+00 0.00000E+00 1.31074E-11 0.00000E+00 14) 4 1.97930E+01 5.61035E+00 0.00000E+00 0.00000£+00 0 000005+00 0 00000E+00 5.83272E-12 5.50989E+00 0.00000E+00 15) - 2 HCO3 CO3= CO2 (ag) CaCO3 (aq) MgCO3 (aq) B(OH)3(aq) B (OH) 4-~ . HS04-OH-3.01685E-09 2.26571E-04 3.09384E-08 3.86103E-04 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1) 0.00000E+00 0.00000E+00 0.00000E+00 1.10196E-07 3.08476E-04 0.00000E+00 0.00000E+00 43 0.000006+00 6 37029E-09 3.82212E-04 2) 25 72976E-07 .09764E-04 .00000£+00 0.0000E+00 0.0000E+00 1.42122E-08 5.79854E~04 2 o 0.00000E+00 0.0000E+00 3) 2.47909E-08 0.0000E+00 7.06447E-04 7.92644E-07 1.46506E~04 0.0000DE+00 0.00000E+00 0.00000E+00 0.00000E+00 2.86004E-06 6.22872E-05 0.0000E+00 0.00000£+00 0.00000E+00 0.00000E+00 10 51 0.000002+00 7.222028-08 8.74979E-04 4.03803E-06 0.00000E+00 67805E-05 .00000E+00 0.00000E+00 0.00000E+00 - 9 1.26379E-06 9.92658E-04 ٥ 0.00000E+00 6) 3.09556E-06 9-99205E-04 1 399978-04 1.65938E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 50 0.00000±+00 0.000002+00 0.00000E+00 0.00000E+00 5 5.30281E-06 2.40670E-04 9.72059E-07 0.00000E+00 8) 0.00000E+00 1.00274E-03 52 0.00000E+00 7.50984E-06 1.00546E-03 41763E-04 6 88224E-07 0.00000E+00 0.00000E+00 0.0000DE+00 0.00000E+00 9) 53 53 0.00000E+00 1.07451E-05 1 00903E-03 4 90734E-04 4.82685E-07 0.00000E+00 0.00000E+00 0.0000E+00 D.00000E+00 10) 1.11397E-03 2.18331£-07 0.00000E+00 0.00000E+00 0.00000E+00 1.02256E-03 0.00000E+00 11) 0.0000E+00 2,40681E-05 00200E-03 :: 0.00000E+00 4.24987E-05 1.04073E-03 .25799E-07 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 12) 54 51 13) 1.01868E-04 1.09867E-03 5 06639E-03 5.533958-08 0.00000E+00 0.00000E+00 0.000000+00 D.00000E+00 0.00000E+00 2,29199E-08 0.00000E+00 0.00000E+00 0.00000E+00 1.64154E-02 0.00000E+00 1.27533E-03 14) 0.00000E+00 2.84255E-04 59 15) 4.83971E-02 1.25492E-08 0.00000E+00 0.00000E+00 0.000002+00 0.00000E+00 0.00000E+00 6.55397E-04 1.63010E-03 55) C ((missing species have zero amounts) €2 NpQ2-Np020H(ag) NDO2 (OH) 2-Np02C03-Np02 (C03) 2=-Np02 (C03) 3==~ Am+++ AmCO3+ Am(CO3)2-1.25197E-16 2.04381E-16 1.33526E-07 1.98384E-11 0.00000E+00 0.00000E+00 0.00000E+00 6.12705E-04 7.72186E-10 373 1) 1.58546E-15 2.55903E-16 1.33573E-07 7.06677E-11 0.00000E+00 0.00000E+00 0.00000E+00 64 1.72085E-04 4.57851E-10 21 65 C0 2.39199E-10 1.81536E-14 0.00000E+00 31 5.08524E-05 3.01827E-10 3.76382E-16 1.33591E-07 0.00000E+00 0.00000E+00 1.33598E-07 5.08355E-10 8.19789E-14 0.00000E+00 0.000002+00 0.00000E+00 5.38926E-16 2.39307E-05 2.47753E-10 41 26769E-15 .33606E-07 1.83431E-09 1.06720E-12 0.00000E+00 0.00000E+00 0.00000E+00 ę. 6.63303E-06 2.00045E-10 1 5) 3.34150E-07 4.20537E-10 0.00000E+00 0.00000E+00 1 76340E-10 1.95555E-14 1.33613E+07 3.641512-08 0.00000E+00 ÷? 33 20 4.75887E-14 1.33616E-07 8.97771E-08 2 .55580£-09 0.00000E+00 0.00000E+00 0.00000E+00 7) 1.35537E-07 1.75190E-10 1.74579E-10 .33620E-07 1.54320E-07 7.55070E-09 0.00000E+00 0.00000E+00 0.00000E+00 7.88495E-08 8.12402E-14 8) ۰. 2.19119E-07 1.52213E-08 0.00000E+00 0.00000E+00 0.00000E+00 91 5.55313E+08 1 74113E-10 1.14749E-13 1.33624E-07 :2 1.63619E-13 1.33630E-07 .145822-07 3.13678E-08 0.00000E+00 0.00000±+00 0.000006+00 10) 3.86794E~08 1.73507E-10 .61801E-13 73 11) 1.70496E-08 1.71249E-10 3 .336548-07 7.13640E-07 1.61308E-07 0.00000E+00 0.00000E+00 0.00000E+00 5.19497E-07 0.000002+00 0.00000E+00 1.28136E-06 0.00000E+00 74. 75 9.49502E-09 1 683168-10 6.28103E-13 1.33688E-07 12) 1.33806E-07 3.23230E-06 3.293698-06 0.00000E+00 0.00000E+00 0.000002+00 1.42922E-12 1,59617E-10 13) 3.76315E-09 1.38078E-10 3.46327E-12 1.34242E-07 1.03462E-05 3.32871E-05 0.00000E+00 0.00000E+00 0.000002+00 /0 12 1.17432E-09 2.94209E-05 2.58546E-04 0.00000E+00 0.0000E+00 0.00000E+00 151 4.11022E-10 1.09291E-10 6.38945E-12 1.35468E-07 73 NDO2OH(amor)_ an (CO3) 3=-Am (OH) 2+ $Am(OR) \exists (a\sigma)$ UO2++ NoO2OH(aged) NaNdO2CO3(s)Na3Np02(C03)2 Th++++ 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 9.99932E+00 0.00000E+00 0.00000E+00 80 1) 0.00000E+00 0.00000E+00 81 52 31 0.00000E+00 0 000002+00 0.00000E+00 0.00000E+00 9.99718£+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 0.0000E+00 0.00000E+00 9.99622E+00 0.00000E+00 31 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 9.99580E+00 0.00000E+00 4) 0.00000E+00 0.000002+00 $\frac{1}{2}$ 0.00000E+00 0.00000E+00 0.00000E+00 0 00000E+00 0.00000E+00 0.00000E+00 9.99531E+00 0.00000E+00 0.00000E+00 0.00000E+D0 0.00000E+00 0.00000E+00 0.00000E+00 e: 2 0 00000E+00 0.00000E+00 0.00000E+00 9.99473E+00 0.00000±+00 0.00000E+00 0.000002+00 0.00000E+00 0.00000E+00 9.99430£+00 0.00000E+00 0.00000E+00 71 0.00000E+00

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27	81	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	
35	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	
fec.	10)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.0000E+00	9.99250E+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	9.98931E+00	0.00000E+00	
		0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.98478E+00		
32	12) 13)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.984/8E+00 9.96914E+00	0.000002+00	
		0.00000E+00	0.00000E+00		0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00		0.00000E+00	
23	14)								9.91117E+00	0.00000E+00	
	15}	0.00000E+00	0.00000E+00	0.00000E+00	0.000002+00	0.00000E+00	0.00000E+00	0.0000E+00	9.74696E+00	0.0000E+00	
<u>e</u> (
4 C		(missing spec	ies have zero a	mounts)							
\$7											
22		IonicStreng		TitrVol,ml	pH	ſ					
03	1)	5.61119E+00	0.00000E+00	0.00000E+00							
	2)	5.61031E+00	0.00000E+00	0.10000	5.6451						
iv i	3)	5.61008E+00	0.00000E+00	0.14251	5.9936						
102	4)	5.61003E+00	D.00000E+00	0.16000	6.2353						
*C:	5}	5.61001E+00	0.00000E+00	0.18000	6.6996						
7 C 4.	6)	5.61006E+00	0.00000E+00	0.20309	7.9427						
- 15	7)	5.61014E+00	0.000002+00	0.22000	8.3317						
*05	8)	5.61024E+00	0.00000±+00	0.24000	8.5655						
107	9)	5.61034E+00	0.00000E+00	0.26000	8.7166						
103	10)	5.61049E+00	0.00000E+00	0.28943	8.8722						
102	11)	5.61112E+00	0.00000E+00	0.41246	9.2225						
1 * * *	12)	5.61202E+00	0.00000E+00	0.58780	9.4695						
/	13)	5.61513E+00	0.00000E+00	1.1938	9.8493						
· · · .	14)	5.62685E+00	0.00000E+00	3.4551	10.295						
113	15)	5.66143E+00	0.00000E+00	10.000	10.659						

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Appendix U: Sample Output File "Np_NaCl_BM_LOG.MOLES"

Appendix U: Sample Output File "Np_NaCl_BM_LOG.MOLES"

See Table 30 for explanation of this listing.

FMT V2.0

5.01.31 A		-OH-C1-C1O4 (NR94)	1
INITIAL and			P91, RFFR92, RFF94, RRFF94)
INITIAL and			
51	INJECTED Abundances 1.1101736300E+02		
Hydrogen	6.1508681500E+01	1.0550868200E+02	
Oxygen Sodium	5.610000000DE+00	1.5610000000E+01	
Potassium	0.000000000E+00	0.0000000000E+00	
Magnesium	0.000000000E+00	0.0000000000E+00	
Calcium	0.000000000E+00	0.000000000E+00	
Chlorine	1.610000000E+00	5.6110000000E+00	
Sulfur	0.0000000000E+00	0.000000000E+00	
Carbon	2.0000000100E+00	1.0000000000E+01	
Posion	0.0000000000E+00 0.000000000E+00	0.0000000000E+00 0.0000000000E+00	
Neglon Air	0.0000000000000000000000000000000000000	0.0000000000E+00	
Boron	0.0000000000E+00	0.0000000000E+00	
Bromine	0.000000000E+00	0.0000000000E+00	
TracerEl	0.000000000E+00	0.000000000E+00	
Th(IV)	0.000000000E+00	0.0000000000E+00	
Am(III)	0.000000000E+00	0.000000000E+00	
U(VI)	0.000000000E+00	0.000000000E+00	
Np(V)	0.00000000E+00	1.000000000E+01	
ClO4-(EL)	0.0000000000E+00 0.000000000E+00	0.000000000000000000000000000000000000	
Phosphorus Electron	0.0000000000E+00	0.0000000000E+00	
Charge	-2.2204460500E-15	-2.3731663200E-15	
0.00.90			
INITIAL and	INJECTED Abundances	AFTER Flashing	
Hydrogen	1.1101736300E+02	1.1101836300E+02	
Oxygen	6.1508681520E+01	1.0550868150E+02	
Sodium	5.6100000000E+00	1.561000000E+01	
Potassium	0.000000000E+00	0.0000000000E+00 0.0000000000E+00	
Magnesium Calcium	0.000000000000000000000000000000000000	0.0000000000E+00	
Chlorine	1.6100000000E+00	5.6110000000E+00	
Sulfur	0.000000000E+00	0.000000000E+00	
Carbon	2.0000000100E+00	1.000000000E+01	
Posion	0.0000000000E+00	0.000000000E+00	
NegIon	0.000000000E+00	0.0000000000E+00	
Air	0.000000000E+00	0.000000000E+00	
Boron	0.0000000000E+00	0.0000000000E+00	
Bromine	0.0000000000E+00 0.0000000000E+00	0.0000000000E+00 0.0000000000E+00	
TracerEl Th(IV)	0.000000000E+00	0.0000000000E+00	
Am(III)	0.0000000000000000000000000000000000000	0.0000000000E+00	
U(VI)	D.000000000E+00	0.000000000E+00	
Np(V)	0.000000000E+00	1.000000000E+01	
C104-(EL)	0.000000000E+00	0.000000000E+00	
Phosphorus	0.000000000E+00	0.000000000E+00	
Electron	0.000000000E+00	0.0000000000E+00	
Charge	-2.2204460493E-15	-2.3731663190E-15	
INITIAL and	INJECTED Concs AFTER	Flashing, molal	
н20			5.5509068E+01
Na+	N	a+ 5.6100000E+00	5.6106128£+00
K+		K+ 0.000000E+00	
		++ 0.000000E+00	0.000000E+00
Ca++			
Mg++			0.000000E+00
Ng++ MgOH+	MgO	H+ 0.000000E+00	0.0000000E+00 0.0000000E+00
Mg++ MgOH+ H+	MgO	H+ 0.0000000E+00 H+ 2.3992707E-12	0.0000000E+00 0.0000000E+00 1.2187250E-06
Mg++ MgOH+ H+ Cl-	мgÖ	H+ 0.0000000E+00 H+ 2.3992707E-12 1- 1.6100000E+00	0.0000000E+00 0.0000000E+00
Mg++ MgOH+ H+ Cl- SO4=	MgO	H+ 0.0000000E+00 H+ 2.3992707E-12 1- 1.6100000E+00 H= 0.000000E+00	0.000000000000 0.000000000000 1.21872500-06 5.61100000000
Mg++ MgOH+ H+ Cl-	MgO C SO HSO	H+ 0.0000000E+00 H+ 2.3992707E-12 1- 1.6100000E+00 H= 0.000000E+00	0.000000E+00 0.000000E+00 1.2187250E-06 5.611000E+00 0.000000E+00
Mg++ MgOH+ H+ Cl- SO4= HSO4-	м ₉ 0 с so нso о нсо	H+ 0.0000000E+00 H+ 2.3592707E-12 1- 1.6100000E+00 4= 0.000000E+00 4- 0.000000E+00 H+ 6.1466486E-03 3- 6.1466639E-03	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO3=	ਸਤੂਹ c so ਸਤਹ ਸ ਮcc ਨਿ	H+ 0.0000000E+00 H+ 2.3592707E+12 1- 1.610000E+00 4= 0.000000E+00 H+ 0.000000E+00 H- 6.146648E-03 3= 6.1466453E-03 3= 1.9938533E+00	0.000000E+00 0.000000E+00 1.2187250E-06 5.611000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.0938611E-08
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO3= CO2 (aq)	н ₉ 0 с с нсо нсо со2 (а	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.0000000E+00 3.0168704E-09 2.2657297E-04 3.0538611E-08 3.8610605E-04
Mg++ MgCH+ H+ Cl- SO4= HSO4- OH- HCO3- CO3= CO2(aq) CaCO3(aq)	н ₉ 0 с so нso нсо нсо со2 (a СаСОЗ (a	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.611000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.0338611E-08 3.8612605E-04 0.0000000E+00
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO3= CO2(aq) CaC03(aq) MgCO3(aq)	н ₉ 0 с с кзо нсо нсо со со со со со со со со со со со со с	H+ 0.0000000E+00 H+ 2.3592707E+12 1- 1.610000E+00 4- 0.0000000E+00 H+ 0.1466486E-03 3- 6.1466439E-03 3- 1.2684969E-03 2.3684969E-09 0.000000E+00 Q1 0.000000E+00 Q2 0.000000E+00	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.0000000E+00 3.0168704E-09 2.2657297E-04 3.0938611E-08 3.8610605E-04 0.0000000E+00
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO2= CO2(aq) CaCO3(aq) MgCO3(aq) B(OH)3(aq)	н уо с с с с с с с с с с с с с с с с с с с	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.611000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.0338611E-08 3.8612605E-04 0.0000000E+00
Mg++ MgOH+ H+ Cl- SQ4= HSQ4- OH- HCQ3- CQ2(aq) CaCQ3(aq) MgCQ3(aq) B(OH)3(aq) B(OH)4-	Hy⊐O C SO HSO CO CO2 (a CaCO3 (a Mg⊂O3 (a B (OH)3 (a B (OH)3 (a B (OH)3 (a	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.8610605E-04 0.0000000E+00 0.0000000E+00
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO2= CO2(aq) CaCO3(aq) MgCO3(aq) B(OH)3(aq)	н уо с с с с с с с с с с с с с с с с с с с	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.0938611E-08 3.8610605E-04 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO2(aq) CaCO3(aq) MgCO3(aq) B(OH)3(aq) B(OH)4- B3O3(OH)4- B3O3(OH)4- CaB(OH)4+	нуо С SO HSO C C C C C C C C C C C C C C C C C C C	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.0938611E-08 3.861065E-04 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
Mg++ MgOH+ H+ Cl- SOd= HSOd- OH- HCO3- CO2(aq) CaCO3(aq) MgCO3(aq) MgCO3(aq) B(OH)3(aq) B(OH)4- B3O3(OH)4- B3O3(OH)4- B4O5(OH)4+	нуо С SO HSO O HCO CO2 (a CCCO3 (a B(OH)3 (a B(OH)3 (a) B3O3 (OH) B3O3 (OH) B3O5 (OH) CaB(OH) MgB(OH)	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.611000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.0338611E-08 3.8612605E-04 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO2(aq) CaCO3(aq) MgCO3(aq) B(OH)3(aq) B(OH)4- B3O3(OR)4- B3O3(OR)4- B3O5(OR)4- CaB(OR)4+ MgB(OH)4+ B3C- B3C- B3C- MgB(OH)4+ MgB(OH)4+ B3C- B3C- B3C- B3C- B3C- B3C- B3C- B3C-	HyO C SO HSO O HSO CO2 (a HCCO3 (a HCCO3 (a B (OH) 3 (a B (OH) 3 (a B (OH) 3 (a B (OH) B 303 (OH) B 405 (OH) C AB (OH) Mg B (OH) B S	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.0938611E-08 3.8610605E-04 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO2(aq) CaCO3(aq) B(OH)3- B(OH)4- B3O3(OR)4- B4O5(OR)4= CaB(OH)4+ Mg8(OH)4+ Br- ClO4-	ну с SO HSO C C C C C C C C C C C C C C C C C C C	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.8510605E-04 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
Mg++ MgOH+ H+ Cl- SO4= HSO4- OH- HCO3- CO2(aq) CaCO3(aq) MgCO3(aq) B(OH)3(aq) B(OH)4- B3O3(OR)4- B3O3(OR)4- B3O3(OR)4+ MgB(OH)4+ Br- ClO4- NaOH(aq)	HyO C SO HSO O HSO CO2 (a HCCO3 (a HCCO3 (a B (OH) 3 (a B (OH) 3 (a B (OH) 3 (a B (OH) B 303 (OH) B 405 (OH) C AB (OH) Mg B (OH) B S	H+ 0.00000000000000000000000000000000000	0.000000E+00 0.000000E+00 1.2187250E-06 5.6110000E+00 0.000000E+00 3.0168704E-09 2.2657297E-04 3.0938611E-08 3.8610605E-04 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00

Appendix U: Sample Output File "Np_NaCl_BM_LOG.MOLES"

Ар	pendix 0. Sample Output File F		LOO.MOLES
8.5	Posion	0.0000000E+00	0.000000E+00
84 84	Negion	0.0000000E+00	0.0000000E+00
¥.	PosIon(OH) (ag)to.titrate.base		0.0000000E+00
25	HNegIon(ag)to.titrate.acid		0.000000E+00
ë T	Tracer(aq)conservative.tracer		0.000000E+00
££	H3PO4 (aq) H3PO4 (aq)		0.000000£+00
23		0.0000000E+00 0.0000000E+00	0.000000E+00
		0.0000000E+00	0.000000E+00 0.0000000E+00
			6.1270920E-04
	NpO20H(ag) NpO20H(ag)	0.0000000E+00	7.7219130E-10
	Np02+ Np02+ Np020H (aq) Np020H (aq) Np02 (OH) 2- Np02 (OH) 2- Np02 (CO3) Np02 (CO3) 2a- Np02 (CO3) 3a=- Np02 (CO3) 3a=-	0.000000£+00	2.0438298E-16
22	Np02C03- Np02C03-	0.000000E+00	1.3352733E-07
25	Np02(C03)2=- Np02(C03)2=-	0.000000E+00	1.9838516E-11
49 • 9	Np02(C03)3==- Np02(C03)3==-	0.0000000E+00 0.0000000E+00	1.2519757E-16 0.0000000E+00
11	Amerit 3mCO3+	0.0000000000000000000000000000000000000	0 0000005+00
:00	Am (CO3)2- Am (CO3)2-	0.000000E+00	0.000000E+00
5.1	Am (CO3) 2 - Am (CO3) 2 - Am (CO3) 3 = - Am (CO3) 3 = - Am (CO3) 3 = - Am (CO3) 3 = - Am (CH) 2 + Am (CH) 2 + Am (CH) 3 (ag) Am (CH) 3 (ag)	0.000000E+00	0.000000E+00
5 V.C	Am(OH)2+ Am(OH)2+	0.000000E+00	0.000000E+00
403 201	Am (OH) 3 (ag) Am (OH) 3 (ag)	0.0000000E+00 0.0000000E+00	0.000000E+00
104 10:			
148	U02++ U(VI)02++ Np020H(aged) Np020H(aged) Np020H(amor) N020H(amor) NaNp02C03(s) NaNp02C03(s)	0.0000000E+00	0.0000000E+00
	NpO2OH(amor)NpO2OH(amor)	0.000000E+00	0.000000E+00
7 (1 5	NaNp02C03 (s)NaNp02C03 (s)	0.0000000E+00	9.9993872E+00
10 ^{6,}	Na3NpO2(CO3)2(s) DISABLED_DISABLED	0.000000E+00	0.000000E+00
	AmOHCO3 (c) AmOHCO3 (c) Am (OH) 3 (s) Am (OH) 3 (s)	0.000000E+00	0.000000E+00
	Am (OH) 3 (s)Am (OH) 3 (s)	0.000000E+00	0.0000000E+00 0.0000000E+00
	AmPO4 (c) AmPO4 (c)	0.0000000000000000000000000000000000000	0.0000000E+00
	NaAm(CO3)2.6H2O(c)AmPO4(c) AmPO4(c)AmPO4(c) CaSO4Anhydrite	0.000000E+00	0.000000E+00
110	NaK3 (SO4) 2Aphthitalite/Glaserite	0.000000E+00	0.000000E+00
1.1.	CaCl2.6H20Antarcticite	0.000000E+00	0.000000E+00
* 2 ** 2	CaCO3Aragonite K2SO4Arcanite MgC12.6H20Bischofite Na2Mg(SO4)2.4H20Bloedite	0.0000000E+00	0.000000E+00
7.3	K2504Arcanite	0.0000000E+00	0.000000E+00 0.0000000E+00
	Na2Mg(SO4)2.4H20 Bloedite	0.0000000E+00	0.0000000E+00
	Mg(OH)2Brucite	0.0000000E+00	0.0000000E+00
102	Mg (OR) 2Brucite Na6CO3 (SO4) 2Burkeite CaCO3Calcite	0.000000E+00	0.000000E+00
122	CaC03Calcite CaC12_4H20CaC12_Tetrahydrite	0.000000E+00	0.000000E+00
2.			0.000000E+00
125 125	Ca4Cl2(0H)6.13H20_Ca0xychloride A Ca2Cl2(0H)2.H20Ca0xychloride B	0.0000008+00	0.0000000E+00 0.0000000E+00
122	KMgCl3.6H20CatoxyChildi lde B KMgCl3.6H20Catrallite MgS04.7H20Dpsomite CaNa2(CO3)2.5H20Gaylussite Na2Ca(SO4)2Glauberite	0.0000000E+00	0.000000E+00
126	MgS04.7H20Epsomite	0.000000E+00	0.000000E+00
128	CaNa2(CO3)2.5H20Gaylussite	0.000000E+00	0.0000000000000000000000000000000000000
132	Na2Ca(SO4)2Glauberite	0.000000E+00	0.000000E+00
7.1	CaSO4.2H20Gypsum	0.000000E+00	0.0000000E+00
102 183	NaCIHalite	0.00000005+00	0.0000000E+00 0.0000000E+00
134	Na2Ca(SO4)2Glauberite CaSO4.2H2OGypsum NaCLHalite MgSO4.6H2OHexahydrite KMCO3Kainite KHCO3Kieserite K2Mg(SO4)2.4H2OKieserite NgSO4.H2OKieserite NgSO4.H2OKieserite NgSO4.H2OKieserite NadCa(SO4)3.2H2OLabile_Salt Marmesite	0.0000000E+00	0.0000000E+00
135	KHCO3Kalicinite	0.000000E+00	0.0000000E+00
	MgS04.H20 Kieserite	0.000000E+00	0.000000E+00
1,7	K2Mg(SO4)2.4H2OLeonite	0.0000000E+00	0.0000000E+00
155 155	Na4Ca(SO4)3.2H2OLabile_Salt	0.0000000E+00	0.0000000E+00 0.0000000E+00
140	MgCO3Magnesite Mg2C1(OH)3.4H2OMgOxychloride	0 0000000000000000000000000000000000000	0.0000000E+00
14:	KHSO4 Mercallite	0.000000E+00	0.0000000E+00
762	KHS04Mercallite Na2504.10H20Mirabilite K8H6(S04)7Misenite	0.000000E+00	0.000000£+00
142	K8H6(SO4)7Misenite	0.000000E+00	0.000000E+00
1.44 1.45	NaHCO3Nahcolite Na2CO3.10H2ONatron	0.0000000E+00	0.000000E+00 0.0000000E+00
140	MgCO3.3H2ONesquehonite	0.0000000E+00 0.0000000E+00	0.0000000E+00
147	K2Mg(SO4)2.6H2O Picromerite/Schoen	0.000000E+00	0.0000000E+00
162	Na2Ca(CO3)2.2H20Pirssonite	0.000000E+00	0.0000000E+00
143	K2MgCa2(SO4)4.2H2OPolyhalite	0.000000E+00	0.000000E+00
150	Ca(OH)2Portlandite K2CO3.3/2H2OPotassium_Carbonate	0.00000002+00	0.0000008+00
101 162	K8H4 (CO3) 6.3H2OPotassium_Carbonate		0.000000E+00 0.0000000E+00
163	KNaCO3.6H20K-Na-Carbonate		0.000000E+00
154	K2NaH(CO3)2.2H20Potassium_Trona	0.0000000E+00	0.000000E+00
155	K3H(SO4)2Sesquipotassium_Sulfate		0.000000E+00
110	Na3H(SO4)2Sesquisodium_Sulfate	0.000000E+00	0.000000E+00
157	Na2CO3.7H20Na2CO3-Heptahydrate	0.0000000E+00 0.0000000E+00	0.0000000E+00
163 159	KC1Sylvite	0.0000000E+00	0.000000E+00 0.000000E+00
142	Mg2CaCl6.12H20 Tachvhvdrite	0.0000000E+00	0.000000E+00
165	K2Ca(SO4)2.H2OSyngenite Mg2CaCl6.12H2OTachyhydrite Na2SO4Thenardite	0.000000E+00	0.000000E+00
· ·	Na2CO3.H2OThermonatrite	0.000000E+00	0.000000E+00
:03	Na3H(CO3)2.2H20Trona Na2B4O7.10H2OBorax	0.000000E+00	0.000000E+00
104 108	Na2B407.10H20Borix_Acid_Solid	0.0000000E+00	0.0000000E+00 0.0000000E+00
14.5	KB508.4H20K-Pentaborate_(30_C)	0.0000000E+00	0.0000000E+00
167	K2B407.4H20K-Tetraborate_(30_C)	0.000000E+00	0.000000E+00
34.8	NaBO2.4H20Sodium_Metaborate	0.000000E+00	0.000000£+00
185	NaB508.5H20Sodium_Pentaborate	0.0000000E+00	0.000000E+00
171	NaBO2.NaCl.2H2OTeepleite_(20_C)	0.000000E+00	0.000000E+00

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Appendix V: Command File FMT_FMTC.COM

Appendix V: Command File FMT_FMTC.COM

```
: 5
               SET noverify
    2.5
                SET verify
    Ş.
                             FMT FMTC.COM assigns and fetches user-selected
    - $ I
                             chemdat and rhomin data base file names,
   0 $1
0 $1
                             assign user-specified imput/output file names,
executes fmt2p0 in CMS 1996 nonPA (Performance
      $!
                             Asssessment) production area
   5.$1
                   •
                              Author: K. M. Aragon
    × $ !
  $
$!
                                                  11/17/95
                              Date:
  : $ $ !
: : : $ !
                              Modifier: S. C. Babb
                              Date:
                                                 12/13/95
  ` $!
  15 $ !
                              Modifier: S. C. Babb
                                               12/18/95
   `>$!
                              Date:
    7$!
                              Reason:
                                                     use fmt executable in production area
                                                    print identity of fmt executable
add log file and mail facility
   3.51
 - . $!
20 $!
21 $!
21 $!
                                                     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
 1:5
 24 $!
 21.51
 20 S!

21 S!

21
 29.51
 20.51
                    Pl - Substring chemdat file name search on valance states, dates,
 21 $1
22 $1
                                     and/or fugacity
  2 s :
                   P2 - Substring rhomin file name search on valance states and/or dates
 24 $1
 (f) $1
                    P3 - Input File Name (no extension)
  20.51
  27 S!-----
2 $2
2 $1
2 $1 Turn on error handling; exit on any error.
4) $1
 21 $
             ON error then goto error_exit
 425
             mode = f$mode()
 ~. $!
43 $1 Logic flow
             GOSUB check_filename
 4 > $
 4.5
             GOSUB define_cms_library
             GOSUE delete files
 <3 S
             GOSUB get_database_files
 ---- S
GOSUB define_inputs
             GOSUB define outputs
 52 $
            GOSUB start_log
\`$! GOSUB start_mail
\'$ GOSUB run_fmt
:: $
: $
             GOSUB undefine_symbols
1°S goto terminate
57 S EXIT
 55 St-----
                                                  ______******
 59 SCHECK_FILENAME:
 5 $! Determine if any or all file names are passed as parameters. If not,
 f $! prompt for one if this is an interactive session;
 \pm 2 $! otherwise flag an error and exit
63.51
 04 S! Check for Pl - this is the CHEMDAT name field
ACS:
CCS IF mode .eqs. "BATCH" .and. pl .eqs. ""
C7S THEN
                    WRITE sysSoutput -
63
                  "Can not run in batch without a chemdat file name (P1). exiting."
SS G
                    GOTO error_exit
 -2 $1
70 $1
74 $ IF pl .eqs. **
73 S
             THEN
 ? > $
.
                     INQUIRE chemdat_name -
                    "Enter chemdat file name to search on
IF chemdat_name .eqs. " THEN goto error_exit
ias
is ellse
i≎s
                     chemdat_name = pl
 SIS ENDIF
 S., $1
5351 Check for P2 - this is the RHCHIN name field
-4 $!
%% IF mode .eqs. "BATCH" .and. p2 .eqs. ""
%% THEN
```

Appendix V: Command File FMT_FMTC.COM

27 **\$** WRITE sys\$output -٤., "Can not run in batch without a rhomin file name (P2). exiting." 94 S GOTO error_exit -: \$ ENDIF ः । \$1 २२ इ। 0 ° \$ IF p2 .eqs. \$ \$ THEN INCUIRE Thomin_name "Enter rhomin file name to Search on" 37.5 IF rhomin_name .eqs. ** THEN goto error_exit 315 ELSE 30 \$ rhomin_name = p2 " 15 \$ THEN WRITE sys\$output -"Can not run in batch without a file name (P3). exiting." GOTO error_exit ENDIF INQUIRE file_name "Enter input file name (without .extension)" IF file_name .eqs. "" THEN goto error_exit
 12 S
 1

 12 S
 1

 12 S
 ELSE

 12 S
 ENDIF
 file_name = p3 1115 RETURN 23 Since Sinc 2 St Define holepa and symmetry
2 St St nonpa_ams_symmetry
22 St Set CMS library to FMT Se \$1 S cms_library_name = fmt* SX S lib cms_library_name 12.51 Set Verify 132.51 133.5 RETURN 135.51-----_____ 55 SDEFINE_INPUTS: 535 \$? Define the input files meeded. 107 \$! 100 \$ DEFINE input 'file_name'.in 13.4 \$ DEFINE inguess 'file_name' inguess id(\$! T4* \$! Define a logical that points to the database files just fetched 142 S 1 143 \$ 144 \$ DEFINE chemdat 'chemdat_name' DEFINE rhomin 'rhomin_name' 14E \$1 148 S RETURN 147 SI %% SDEFINE_CUTPUTS: %% \$! Define the output files needed. 10. S. 18:5 DEFINE output 'file_name'.out
16:2 DEFINE for088 'file_name'.for088
16:3 DEFINE titrate 'file_name'.titrate 164 \$ 165 \$! DEFINE moles 'file_name'.moles 108 S RETURN 187 51-----STELETE_FILES: :∹3 **\$**1 101 **5**1 100 \$: 522 \$ SET noon 102 \$ SET message/nofac/nosev/notext/noid 104 \$! Delete all 'file_name'.moles files; do not accumulate them. 145 S! 145 S DELETE 'file_name'.moles;* "07.5: Delete all fmt prefixed files of chemdat and rhomin files "08.5! 1825 1825 1725 1725 DELETE fmt_*.chemdat;* DELETE fmt_*.rhomin;* SET message/fac/sev/text/id SET on 175 **S** ! 176.5 RETURN 128 \$!--______ SERROR_EXIT:



Appendix V: Command File FMT_FMTC.COM

WW \$! Exit routine when a severe error is encountered 17% \$1 17% \$1 17% \$ Write sysSoutput "Executing error exit, ''\$status'." 10% \$ EXIT 10: 5:-----16. SGET_DATABASE_FILES: The S! If interactive, allow user to select/pick from a list of chemdat file names 195.51 SSC S IF mode .nes. "BATCH" ST\$ THEN cse **''chemdat_name'*.chemdat" 1103 5 S-2 \$ 1 _INQUIRE chemdat_name "Select CHEMDAT name from list above" 190 **\$** S ENDIF 102.51 "D: S: Fetch chemdat from FMT CMS Sec. 51 :::: \$! set noverify '39 \$ cfe 'chemdar_name'
'0? \$! set verify 103 \$1 30-51 If interactive allow user to select/pick from a list of rhomin file names 20051 2015 IF mode .nes. "BATCH" SC S THEN 20% \$ cse **''rhomin_name'*,rhomin* 204 \$1 208 s INQUIRE rhomin_name "Select RHOMIN name from list above" 208 S ENDIF 2.7 \$1 2005 \$! Fetch chemdat from FMT CMS 209 S: set noverify 201 S cfe 'rhomin_name 203 S: set verify 272 51 215 SRUN_FMT: CCS: Define the run symbols needed.
 C/7 \$
 define /nolog exe_dir
 wp\$nonpa_

 fmt2p0
 :== *\$exe_dir:fmt_fmt2p0_pa96.exe*
 wp\$nonpa_prodroot:[fmt.exe] 213 \$1 2005; Run the utility that shows image information from the exe. (mandatory!) 2005; St This is part of the documentation required while doing a calculation. 2005 & @wpSref:wp_get_image_id.com exe_dir:fmt_fmt2p0_pa96.exe 223 St Run the code 224 \$1 225 \$ fmt2p0 276 \$ RETURN 227 \$1-----______ SAN SSTART_LOG 228 \$1 260 s month == f\$cvtime('''f\$time()'', 'absolute', 'month') day == fsctime(''f\$time()'', 'comparison', 'day')
hour == f\$cvtime(''f\$time()'', 'absolute', 'hour')
min == f\$cvtime('''f\$time()'', 'absolute', 'minute') 255.5 Zoc S hour 283 \$ 284 \$ F min 201 S log_file_name :== *''file_name'_''month'''day'_''hour'''min'.log* 203 S! mike williamson's log file definition: 203 S! "sysSlogin:fmt_''file_name'_''month'''day'_''hour'''min'.log* 203 S! "sysSlogin:fmt_''file_name'_''month'''day'_''hour'''min'.log* 235 \$1 205 \$ DEFINE/proc sys\$output 'log_file_name 241 S RETURN 262 \$1----_____ 243 SSTART MAIL: 2^{243} S! Open a file where we can write a message that can be sent to the 245 \$! user upon completion. 245 \$: 247 \$ mail_error_flag = 0 240 \$ mail_file_name :== *sys\$Login:fmt_mail.msg* 243 \$ mail_subject :== *FMT ''file_name' run.* 250 \$ mail_list == f\$getjpi(**, *username*) 200 S mail_Subject ... Fail file_name
200 S mail_list == fSgetjpi('', 'username'
201 S!
202 S OPEN/write mail_file 'mail_file_name 283 \$1 254 S RETURN 243 200 \$!-----200 \$! If there was no previously flagged error or problem, search the log files 200 \$! for any fatal, error, or warning messages. 240 **\$**1 201 \$! Deassign sysSoutput so the 'log' file closes. 71- \$ deassign sys\$output 223 \$1 30% \$! Show the run output to the user 201 \$ TYPE 'log_file_name 201 \$!

Appendix V: Command File FMT_FMTC.COM

••
207 St Skip sending the mail message
205 \$ goto end_terminate
200 51
370 S! If there was not a previous error recorded, search the log file for
27:\$! common error indicators.
272\$ search_status = 0
273 \$ IF mail_error_flag .ne. 1
274 \$ THEN
275 \$: Turn off informational messages from search command
276 \$ SET message/nofac/nosev/notext/noid
277\$ SEARCH 'log_file_name '-F-','-E-','-W-' / match=or
278 \$ search_status = \$status
273 \$! Turn on messages
260 \$ SET message/fac/sev/text/id
2015 ENDIF
032.\$1
292 \$ IF search_status .eq. 1 .or. mail_error_flag .eq. 1
284 \$ THEN
200 \$ WRITE mail_file "The run log contains an error or warning."
<pre>200 \$ WRITE mail_file "Please examine ''log_file_name'." 207 \$ mail_subject == "''mail_subject' ERROR"</pre>
223 \$ WRITE mail_file "The FMT run has completed." 293 \$ ENDIF
295 St
240 S CLOSE/nolog mail_file
<pre>293.5 MAIL/subject="''mail_subject'' 'mail_file_name 'mail_list</pre>
DOE SEND_TERMINATE:
296 \$ EXIT
297 \$}
293 SUNDEFINE_SYMBOLS:
200\$! Deassign input files
900 \$1
303 \$ DEASSIGN input
102 \$ DEASSIGN inquess
State DEASSIGN chemdat
생각 S DEASSIGN rhomin 2022 S DEASSIGN output
SOUS DEASSIGN FOR 088
307.5 DEASSIGN FOLVOO
See S Deassier cleare
312 S RETURN
/ 1 St
3 2 S: CMS REPLACEMENT HISTORY, Element FMT_FMTC.COM
3735! *2 21-DEC-1995 12:58:57 SCBABB *FMT EXECUTABLE NAME CHANGED*
314 \$! *1 19-DEC-1995 12:26:54 \$CBABB *USER COMMAND FILE FOR EXECUTING FMT_FMT2PO FROM CMS*
215 \$! CMS REPLACEMENT HISTORY, Element FMT_FMTC.COM

 \sim

Appendix W: Review Forms

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



NOTE: Copies of the User's Manual Reviewer's Forms are available in the Sandia WIPP Central Files.