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Leachate Contaminant Reduction Time Study

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Concentrations of selected design inventory constituents in INEEL CERCLA Disposal Facility (ICDF) landfill leachate were evaluated to estimate leachate chemical characteristics during the 15-year operations period and the 30-year post-closure period. The purpose of the study was to estimate leachate constituent concentrations to support various design evaluations including:

- Identifying a conservative estimate of the leachate chemical characteristics as a basis for assessment of landfill liner/leachate compatibility;
- Identifying a conservative estimate of the leachate chemical composition to assess worker exposure to landfill contaminants in the leachate evaporation ponds.

Three approaches were taken to evaluate the leachate as described below:

1. To identify potential maximum leachate concentrations in the landfill, a geochemical model was used to simulate the chemical nature of the leachate at the approximate moisture content of the compacted waste soil.
2. To identify the potential loss of constituents from the waste soil in leachate during the 15-year operating period, a spreadsheet-based analytical solution was used.
3. To identify potential concentration of leachate constituents outside of the landfill during the 30-year post-closure period, a numerical simulation model (i.e., STOMP, the same model used for fate and transport simulations to evaluate groundwater remedial action objectives) was used to estimate the volume and characteristics of the leachate.

The geochemical modeling indicates that pore water within the compacted waste soil is expected to be a brackish to saline water (approximately 0.5 molar ionic strength) dominated by sodium and sulfate and buffered by carbonates to a pH of around 8.0. The analytical solution indicates that as much as 20% of the inventory masses of the most mobile constituents (e.g., iodine and technetium) may be removed from the landfill during the 15-year operation period. The numerical simulations of constituent transport during the 30-year post-closure period indicated that less than 1% of the contaminant mass would be expected to leave the landfill as leachate during the post-closure period. Because of the high degree of uncertainty regarding the actual rate of waste soil placement in the landfill and the actual placement of specific waste soil, conservative assumptions were made that are believed to maximize apparent leachate concentrations for these evaluations.

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ABSTRACT

Concentrations of the design inventory constituents in the INEEL CERCLA Disposal Facility landfill leachate were simulated over the 15-year operations period and 30-year post-closure period. The purpose of the study was to examine the chemical nature of the leachate and the change in leachate concentration over time. The results provide a basis for assessment of leachate/liner compatibility, and also support evaluation of worker exposure to waste constituents that may be present in the facility leachate evaporation ponds. Three approaches were taken to evaluate the leachate.

1. A geochemical model was used to predict the general chemical characteristics of the leachate. A group of design inventory constituents screened on the basis of concentration and representing 99% of the total mass were equilibrated with pore water within the compacted waste soil in the landfill. The leachate is predicted to be a brackish to saline water dominated by sodium and sulfate with ionic strength of approximately 0.5 molar and buffered by carbonates to a pH of around 8.0. The modeled pore water concentrations provide the most conservative basis for liner compatibility evaluation.

2. A spreadsheet calculation was used to estimate potential landfill design inventory constituents removed from the landfill during the 15-year operating period. The spreadsheet calculation simulated partitioning to the solid phase via adsorption, radioactive decay, and leachate removal from the landfill. The results indicate as much as 20% of the inventory masses of the most mobile constituents (e.g., tritium and iodine), about 5% of the technetium-99, and less than 1% of the uranium isotopes and neptunium-237 are expected to be removed from the landfill during the operation period.

3. The STOMP model was used to simulate potential landfill design inventory constituents removed from the landfill during the anticipated 30-year post-closure period with the final cover in place. The results of the 30-year post-closure transport simulation indicate less than 1% of the inventory masses of even the most mobile constituents are expected to be removed from the landfill during the post-closure period (i.e., following placement of the final cover).

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ACRONYMS

CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
DAF	dilution/attenuation factors
EDF	engineering design file
HDPE	high-density polyethylene
ICDF	INEEL CERCLA Disposal Facility
INEEL	Idaho National Engineering and Environmental Laboratory
PNNL	Pacific Northwest National Laboratory
STOMP	subsurface transport over multiple phase
USGS	U.S. Geological Survey

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Leachate Contaminant Reduction Time Study

1. INTRODUCTION

The purpose of the Leachate/Contaminant Reduction Time Study is to document the estimated composition of both the leachate and the landfill waste soil mass over the periods of operation (15 years) and post closure (30 years) at the Idaho National Engineering and Environmental Laboratory's (INEEL) proposed INEEL CERCLA Disposal Facility (ICDF) landfill. During operation and post-closure periods, the leachate will flow through the leachate collection system and will be discharged to the evaporation pond. Results of this study will be used to evaluate compatibility of the synthetic and natural liner components with the leachate and to estimate pond water composition over time to support other assessments.

The evaluations are conducted separately based on the operations period (using two different approaches) and the post-closure period (using one method). For the operation period, the leachate concentrations were simulated using both a geochemical model (Section 2) and a spreadsheet-based analytical solution method (Section 3). For the subsequent 30-year post-closure period, a numerical simulation was performed using the Subsurface Transport Over Multiple Phases (STOMP) code, assuming placement of the final cover (Section 4).

The geochemical model was used solely to predict general chemical characteristics of the leachate for later use in the leaching transport models. Because of the voluminous list of constituents, the geochemical modeling screened the design inventory elements down to those that account for greater than 99% of the total mass identified in the design inventory. Section 2 provides a detailed description, assumptions, and results of this evaluation.

The spreadsheet-based analytical solution was used to estimate the potential landfill design inventory constituents removed from the landfill during the 15-year operation period. This evaluation partitioned the design inventory mass of all of the contaminants of concern between soil and leachate aqueous concentrations on the basis of partitioning coefficients (which are used to estimate the degree of adsorption to soil mineral surfaces). The spreadsheet-based analytical solution did not account for or include any solubility limitations. Leaching rates were applied, along with radioactive decay rates (where applicable) to determine the possible mass removal from the landfill over time. Plots were constructed of potential landfill mass concentrations and landfill leachate concentrations over time during the 15-year operating period. Section 3 provides a detailed description, assumptions, and results of this evaluation.

The STOMP simulation, a numerical simulation of the 30-year post-closure period with the final cover in place, also included the entire design inventory mass of all of the contaminants of concern. The model grid and construction was a subset of the model described in EDF-ER-275 that included the waste and operations layers. The top of the clay layer, where the liner system functions to prevent downward flow, was set to act as a no-flow boundary. Two numerical seepage face boundaries on top of the clay layer and on both sides of the ICDF model domain provided the means to evaluate the flow and contaminants exiting the model. Section 4 provides a detailed description, assumptions, and results of this evaluation.

Details regarding constituent screening, calculations, simulations, and modeling results used in this study are provided in the following appendices:

- Appendix A—Constituent Solubility Modeled Using PHREEQC
- Appendix B—PHREEQC Input and Output Files

- Appendix C—Leachate Generation Calculations 15-Year Operations Period
- Appendix D—Leachate Concentration Estimates for the 30-Year Post-Closure Period
- Appendix E—PHREEQC Constituent Screening
- Appendix F—Analysis of Leachate Reduction for the ICDF Landfill and Evaporating Ponds.

2. GEOCHEMICAL MODELING

The geochemical model was used to predict the general chemical ch4aracteristics of the leachate. A group of the design inventory was screened to identify major constituents for geochemical modeling. Because the geochemical modeling activity is computationally intensive, individual constituents accounting for less than 0.01% of the design inventory were excluded from the geochemical modeling activity. The retained constituents account for more than 99.9% of the contaminant mass identified in the design inventory. Additional details regarding the screening are provided in Section 2.1 and Appendix E.

2.1 Screening Process

Initial activities included the screening of constituents. Quantities of inorganic (non-radioactive) and organic compounds were reported as total kilograms (kg), whereas concentrations of radionuclides were provided as total curies in the "INEEL CERCLA Disposal Facility Design Inventory" (EDF-ER-264). These were converted to kg using published half-lives and atomic mass for each isotope. For elements with reported concentrations of radioactive and non-radioactive forms, the isotope masses were summed, although in these cases the radioactive concentrations were far less than those of non-radioactive isotopes. The source of radioactive constitue4nts was Table D-3 from the design inventory (EDF-ER-264).

The screening process is illustrated in Figure 1. Two screening exercises were completed. The first was based solely on partition coefficient (K_d) values. As 4shown on the portion of Figure 1 marked "1", all elements with K_d values less than 20 were considered significantly leachable during the operations period and were therefore included in the leachate generation calculations presented in Section 4. A K_d of 20 corresponds to 1% of the waste mass leaching into solution. These constituents were assumed to have no solubility controls, and were assumed to partition to the aqueous phase according to their K_d values. The resulting list of elements, including their milligrams per kilogram (mg/kg) concentrations, K_d values, and corresponding aqueous concentrations, is provided in Appendix E as Table E - 1. The constituents with K_d values greater than 20 are displayed in Table E-2.

The second screening exercise (marked "2" on Figure 1) was based on the nature and concentration of inventory constituents. All constituents existing in solution as anions were included, regardless of their concentrations in the inventory. Plutonium is predominantly in anionic form above pH 8, and uranium carbonate species are anionic, so both of these elements were included, even though they are assumed to be cations in many studies. Organic compounds were assumed to be neutral species. All inventory organics were eliminated because none was over 1% of the total mass fraction, calculated by dividing the total kg for a given compound by the assumed total waste stream mass of 5.85×10^8 kg. Inorganic constituents were screened to include only those that constituted over 0.01% of the total mass fraction. Since there is a minimal amount of organic constituents in the design inventory, 1% was selected as the criteria to identify the major chemical species contributing to the leachate chemistry. Similar screening was used for the inorganic species with the intent to identi4fy the species that contribute 99.99% of the constituents in the leachate. The final list of constituents for this screening exercise is shown in Appendix E as Table E-3. Those constituents that were screened out are provided in Table E-4.

The second list was included in a geochemical model to correct for solubility in the leachate before being passed to the leachate generation calculations.

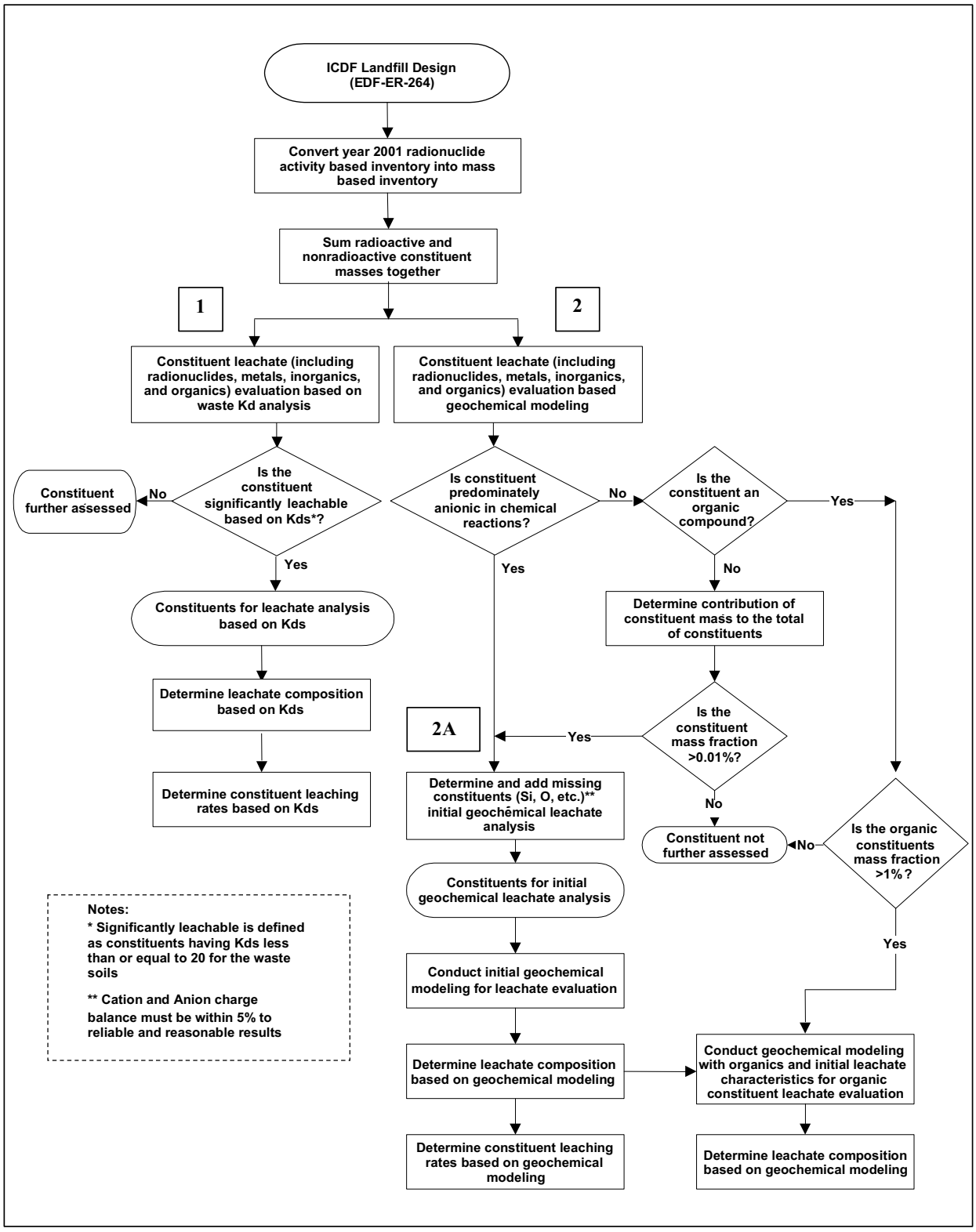

Figure 1. Screening process flowchart for geochemical evaluations.

2.2 General Principles

The geochemical model PHREEQC, v. 2.5 (Parkhurst and Appelo 1999), was used for this study, using a recently released database, LLNL.DAT, which contains species and mineral phase data for all of the screened elements. PHREEQC receives as input all aqueous concentrations of constituents in the infiltrating water, along with quantities of all mineral phases believed to be present in the landfill material. Geochemical conditions are also specified, namely the pH, redox potential, and the presence of atmospheric gases (O_2, CO_2, etc.). These conditions may either be set or allowed to change as the system equilibrates.

The model takes into account all elements reported and, using the database, calculates concentrations and activities (concentrations corrected for ionic strength) of all aqueous species present. For example, calcium exists in various aqueous forms including Ca^{2+}, $CaHCO_3^+$, $CaCl^+$, etc. Saturation with respect to applicable mineral phases is also calculated by comparing the ion activity product with the solubility product constant (K_{sp}) for a given mineral. For example, the mineral calcite ($CaCO_3$) has a K_{sp} of approximately $10^{-8.4}$. This means that under equilibrium conditions, the product of the aqueous activities of the ions Ca^{2+} and CO_3^{2-} is $10^{-8.4}$. If this product is greater than the K_{sp}, the solution is said to be supersaturated with respect to calcite, and undersaturated if the opposite is true. This demonstrates the importance of calculating the free concentration of mineral constituent ions such as Ca^{2+}. Other ions in solution may complex Ca^{2+} or reduce its activity by contributing to higher ionic strength. PHREEQC calculates these effects for all input elements and minerals.

One of the many other features of the PHREEQC model is the ability of the user to assign equilibrium conditions to selected mineral phases. In this way, if minerals are known or suspected to exist at a site, the user may instruct PHREEQC to dissolve the necessary amounts of those minerals to achieve equilibrium with the surrounding solution. This feature was used in the present study.

2.3 Site-Specific Methodology

The first step in the geochemical model setup was to input the infiltrating water chemistry. The average annual rainfall at the site was assumed to be approximately 8 in./yr (NOAA 1989). In addition, site water supplies will be used for dust suppression and compaction during the operating period at an estimated rate of 10,000 gallons per week (EDF-ER-269). This corresponds to an equivalent of 1.43 in./yr in applied water. The infiltrating water will therefore have a proportion of 85% rainwater and 15% applied water. Major chemical constituents for each water source were input to PHREEQC, using an average rainwater analysis (Brownlow 1996) and site records for Well CPP-1.[a] The two waters were mixed in the proportions described above and the resulting solution was saved for further modeling. In a later sensitivity analysis, the applied water was doubled to 20,000 gallons per week and there was virtually no change in the final model results (described below).

It was assumed that this soil moisture content will be 6% by weight during the operations period (DOE-ID 2000). Further, assuming 1 kg of applied water corresponds to 1 liter, each liter of leachate would be exposed to 16.7 kg of landfill soil. In the geochemical model, 1 liter of the water mixture described above was equilibrated with specified molar quantities of minerals present in 16.7 kg of soil.

The second step of the geochemical modeling was to assign mineral phases to site soil and/or controls on constituent solubility. Mineralogy (with average percent abundance) reported in soils on the Chemical Processing Plant consisted of quartz, plagioclase feldspar, potassium feldspar, calcite,

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a. Provided by Marty Doornbos in a personal communication to CH2M HILL, 2001.

pyroxene, and detrital mica (USGS 1989). Simplifying assumptions were made to assign specific minerals to plagioclase (albite), potassium feldspar (orthoclase), pyroxene (enstatite), and mica (illite). The average percent abundance of each mineral was converted to g/kg with the assumption that the minerals have approximately equal density. The g/kg concentrations were converted to total grams by multiplying by 16.7, the total kg exposed to each liter of leachate (see above). Finally, the grams of each mineral were converted to moles by dividing by the molecular weight of each mineral. The calculations are summarized in Table 1.

Table 1. Calculation of mineral abundance in site soils.

	Quartz	Albite (plagioclase feldspar)	Orthoclase (potassium feldspar)	Calcite	Enstatite (pyroxene)	Illite (mica)
Average abundance (%)[a]	38.3	22.7	13	3.7	13	9.3
g/kg soil	383	227	130	37	130	93
mineral molar mass (g/mol)	60	262	278	100	100	383.5
mol/kg soil	6.39	0.87	0.47	0.37	1.30	0.24
mol exposed to 1 L leachate[b]	39.5	5.3	2.9	2.3	8.0	1.5

a. Average of BLRB-7, BLRB-8, and BLRB-9 (USGS 1989).

b. Calculated by multiplying mol/kg by 6.18 kg soil per L void space (see text).

Some of the soil minerals listed above are typically not in direct equilibrium with pore water in natural environments. Feldspars will have a microscopic layer of clay mineral on the weathering surface. Though minute in overall mass concentration, this clay mineral (kaolinite was assigned for modeling purposes) controls the aqueous concentrations of aluminum and silicon. As magnesium-rich minerals such as enstatite dissolve, the aqueous concentration of magnesium is typically controlled by dolomite in this environment. Kaolinite and dolomite were input to PHREEQC only as solubility controls, not as quantified masses.

Inventory elements not accounted for by the calculations in Table 2-1 were assigned to realistic solid phases based on the geochemical environment (i.e., oxidizing, neutral to slightly alkaline conditions). Metal cations were commonly assigned oxides, hydroxides, or carbonates that form in near-surface regimes. Although not expected in oxidizing environments, significant sulfide was reported in the inventory. To account for this mass, the common sulfide minerals pyrite (FeS_2) and sphalerite (ZnS) were included. In a soil environment open to the atmosphere such as this one, equilibrium calculations predict that all sulfides will be oxidized to sulfate and dissolve. Zincite ($ZnCO_3$) was used as a control on zinc solubility, and ferric hydroxide ($Fe(OH)_3$) was used both as a source of iron and a control on its solubility. A list of the screened elements and their mineral source(s) and control(s) is provided in Appendix A as Table A-5. Some design inventory contaminants will likely exist in soluble solid forms such as sodium salts. During water infiltration they would dissolve and reprecipitate as the modeled phases described above. To eliminate guessing the solid forms in the waste stream, the modeling was accomplished by assigning the stable solid phases and calculating the concentration of the solution in equilibrium with these phases.

Two very soluble anions, cyanide (CN^-) and iodide (I^-), were not represented by realistic minerals in the LLNL database. To account for these constituents, they were added as sodium salts under the reasonable assumption of complete dissolution.

One liter of the infiltrating water mixture was equilibrated with the molar quantities of the minerals listed in Table A-5. Because the system is open to the atmosphere during the operating period, the system was also equilibrated with atmospheric oxygen (P_{O2} = 0.2 atm) and carbon dioxide ($P_{CO2} = 10^{-3.5}$ atm). Redox potential was calculated on the basis of oxygen fugacity and pH was calculated as part of the equilibration process.

2.4 Results of Geochemical Modeling

The modeled concentrations of the screened elements are reported in Table 2. The complete PHREEQC input and output files are provided in Appendix B. The modeled leachate is a brackish water (total dissolved solids around 46,000 mg/L) dominated by sodium and sulfate with a pH of 8.0. The water chemistry is most influenced by the oxidation of sulfide minerals, equilibration of carbonates, and dissolution of the more plentiful of the soluble components of the design inventory (such as boron, phosphorus, terbium, vanadium, and ytterbium, along with the major elements).

Elements that were only slightly soluble included barium, zinc, plutonium, and uranium. Salts of most anionic constituents were completely dissolved before equilibration could be reached. These constituents included chloride, iodide, technetium, selenium, and arsenic.

These results represent an approximation of chemical conditions. The mineral phases were chosen on the basis of the best available data and what were considered reasonable assumptions regarding the geochemical environment. As discussed above, the model predicted complete oxidation of sulfide due to the equilibration condition with atmospheric oxygen. This process may be limited during the operation period by chemical kinetics, but insufficient data were available for quantification.

Partition coefficients (K_d values) were not applied during the geochemical modeling stage. The leachate generation calculations described in Section 3 involved application of K_d values and radioactive decay.

Table 2. Results of PHREEQC simulation: calculated constituent concentrations in leachate (no partitioning applied).

	Constituent	mol/kg H2O[a]	mol/L	Molar Mass	mg/L
Aluminum	Al	5.29E - 08	4.97E - 08	26.98	1.3E - 03
Arsenic	As	1.28E - 03	1.20E - 03	74.9	9.0E + 01
Boron	B	2.46E - 01	2.31E - 01	10.8	2.5E + 03
Barium	Ba	2.05E - 08	1.92E - 08	137	2.6E - 03
Carbon (rad) [b]	C		not calculated	14	6.4E - 11
Carbon (non-rad)	C	6.69E - 02	6.28E - 02	12	7.5E + 02
Calcium	Ca	1.09E - 02	1.03E - 02	40	4.1E + 02
Chlorine	Cl	1.14E - 03	1.07E - 03	35.5	3.8E + 01
Fluoride	F	1.28E - 03	1.20E - 03	19	2.3E + 01
Iron	Fe	4.66E - 07	4.38E - 07	55.847	2.4E - 02
Iodine (rad)	I	1.01E - 06	9.49E - 07	129	1.2E - 01
Potassium	K	3.56E - 04	3.35E - 04	39.1	1.3E + 01
Magnesium	Mg	9.26E - 04	8.70E - 04	24.3	2.1E + 01
Manganese	Mn	6.06E - 13	5.70E - 13	54.9	3.1E - 08

Table 2. (continued).

	Constituent	mol/kg H2O[a]	mol/L	Molar Mass	mg/L
Sodium	Na	3.63E - 01	3.41E - 01	23	7.8E + 03
Nitrate	NO3	1.29E - 03	1.22E - 03	62	7.5E + 01
Phosphorus	P	3.83E - 03	3.60E - 03	31	1.1E + 02
Plutonium (rad)	Pu	3.09E - 13	2.90E - 13	244	7.1E - 08
Selenium	Se	1.92E - 04	1.80E - 04	79	1.4E + 01
Sulfate	SO4	2.24E - 01	2.10E - 01	96	2.0E + 04
Tellurium (rad) b	Te		not calculated	128	1.5E - 10
Silicon	Si	1.07E - 04	1.00E - 04	28	2.8E + 00
Terbium	Tb	6.39E - 02	6.00E - 02	158.9	9.5E + 03
Technitium (rad)	Tc	6.09E - 08	5.72E - 08	98.9	5.7E - 03
Uranium (rad)	U	3.63E - 06	3.41E - 06	238	8.1E - 01
Vanadium	V	7.45E - 03	7.00E - 03	50.9	3.6E + 02
Ytterbium	Yb	2.00E - 02	1.88E - 02	173	3.3E + 03
Zinc	Zn	1.29E - 04	1.21E - 04	65.4	7.9E + 00

a. Due to dissolution of significant quantities of mineral phases, the density of leachate is calculated to be 1.064 kg/L

b. These constituents were not modeled in PHREEQC; concentration represents complete dissolution.

3. LEACHATE GENERATION RATE AND CONTAMINANT REDUCTION OVER TIME

Application of partitioning coefficients (K_d values) to the design inventory mass estimates was used to evaluate the contaminant mass adsorbed to the soil and the mass contained in the aqueous phase. The resulting concentrations were then determined on the basis of the total mass of soil estimated to be disposed in the landfill, and the design moisture content, respectively. Annual leachate losses, combined with radioactive and environmental decay, were used to calculate changes in leachate and landfill composition over the operating period. The methodology and results for each group are presented below.

3.1 Leachate Generation

3.1.1 Introduction

An analytical solution was applied to estimate the loss of the design inventory contaminants from the emplaced waste in the ICDF during the period of time that the landfill is in operation and prior to placement of the final cover. This model is intended to support decisions regarding waste placement and to facilitate understanding of the mobility of contaminants within the facility. The approach and methodology used in this evaluation are described in the following sections.

3.1.2 Approach

An analytical model utilizing Microsoft Excel™ spreadsheet tools was prepared. The spreadsheet format allows rapid development of the model and ease of modification of specific input parameters to support sensitivity analyses. Input to the model includes the ICDF design inventory for contaminants, estimated waste mass and volume, and project-specific distribution/partition coefficients (Kd) for site

contaminants. The model utilizes simplified assumptions regarding moisture content of the waste soil within the landfill and water recharge through the emplaced waste. The details of the model methodology are described in Section 3.1.3.

3.1.3 Methodology

The inventory and release model estimated the concentration of each contaminant in the leachate exiting the ICDF yearly, and the amount of contaminant mass remaining within the ICDF. These parameters were modeled over a 15-year period during which the landfill is assumed to be filled to capacity and before placement of the cover. The model assumptions and computational details are described in the following subsections.

3.1.3.1 Assumptions. The following assumptions were applied to support development of the analytical model:

- The landfill was assumed to be filled to capacity at the start of the computations (i.e., the design volume of waste soil is in place at time zero [T0], or the start of the simulation).
- The uniform waste soil moisture is assumed to be 6% by weight (DOE-ID 2000) at the beginning of the simulation, and remain unchanged during the 15-year period.
- The initial leachate concentration was assumed to be the contaminant mass present in the design inventory, distributed between the solid and solution phases according to the site-specific distribution coefficients (Kd).
- All contaminants of concern were included in the simulation.
- Contaminant mass leaves the landfill only by leachate transport and/or by radioactive or environmental decay, as applicable.

3.1.3.2 Computations. Contaminant mass exited the ICDF only by means of leachate transport and/or radioactive or environmental decay. The model essentially consisted of determining the equilibrium concentration of each contaminant in solution and on solids contained within the ICDF, and then calculating the amount of leachate exiting the ICDF. Thus, the amount of contaminant remaining in the ICDF equaled the initial mass minus the mass transported by the leachate and the mass lost to radioactive decay.

Beginning with the initial inventory for each contaminant, the total mass (m_T) equaled the mass of contaminant on the solids (m_s) and the mass of contaminant in solution (m_{aq}):

$$m_T = m_s + m_{aq} \quad or \quad m_T = c_s M + c_{aq} V \tag{1}$$

where

The contaminant concentration on the solids (cs) equals the mass of the contaminant on the solids divided by the total mass content of the ICDF (M), and the contaminant concentration in solution (caq) equals the mass of contaminant in solution divided by the total water content of the ICDF (V). The ICDF moisture content of 6% by weight was assumed at the start of the simulation time with no change occurring in the water content. At equilibrium, the distribution coefficient (kd)

equals the ratio the contaminant concentration on the solids to the contaminant concentration in solution:

$$k_d = \frac{c_s}{c_{aq}} \tag{2}$$

Combining the two equations results in the following relationships:

$$c_{aq} = \frac{m_T}{(k_d M + V)} \quad and \quad c_s = k_d c_{aq} \tag{3}$$

The mass of contaminant exiting the ICDF each year equals the leachate concentration multiplied by the leachate volume (v_i), and the mass remaining (m_{Ti+1}) is the initial mass minus the leachate mass, less the mass lost to radioactive or environmental decay:

$$m_{Ti+1} = m_{Ti} * e^{-\ln(2)/T_{1/2}} - c_{aq} v_i \tag{4}$$

where

T1/2 is the half-life of the radioactive isotope or organic compound. For non-decaying contaminants (T1/2 = 0), the exponential term equals 1. The contaminant concentrations for the following year are then calculated using the remaining total mass, and the preceding contaminant concentration equations.

3.1.3.3 Model Input Parameters. The naturally occurring background recharge for the INEEL site is estimated to be 1.0 centimeters (cm) per year. Because of the trapezoidal shape of the landfill, estimated water recharge through the landfill waste mass was increased according to the ratio of the top of the landfill to the bottom of the landfill (1.74:1, see Section 4.1.3 for a complete explanation). Thus the simulation was performed using a recharge rate of 1.74 cm per year or 0.0174 m/yr.

The initial mass of moisture in the landfill equals the moisture content (by weight) multiplied by the mass of soil in the landfill. The design inventory is 5.85E + 08 kg of waste, so the initial mass of water is 3.51E + 07 kg of water. At an assumed water density of 1.0 kg/L, the initial volume of water equals 3.51E + 07 L. The volume of water exiting the landfill each year equals the ratioed recharge rate multiplied by the area of the bottom of the landfill (0.0174 m/yr * 160 m * 194 m): 5.40E + 02 m^3/yr or 5.40E + 05 L/yr.

3.1.4 Simulation Output and Discussion

Concentrations of all constituents from Table A-1 were calculated for each year of the operation period, and the results are presented in Appendix C of this report. The leachate reduction simulation indicates that contaminant mass reduction due to leaching of selected highly mobile contaminants (i.e., iodine-129 and tritium, technetium-99, and neptunium-237) is typically around 20% of the design inventory mass over the 15-year simulation period at the background recharge rate. Iodine-129 was assigned a K_d of zero, and therefore represents the most conservative conditions. Technitium-99 has a K_d value of 0.2 ml/g and experienced a contaminant reduction of approximately 5%. The uranium isotopes and neptunium-237 have K_d values of 6.0 and 8.0 ml/g, respectively, and experienced contaminant reductions of less than 1%. The leachate concentration and residual contaminant mass for the selected iodine, technetium, and neptunium isotopes for the 15-year simulation period at the 1.0 cm/yr recharge rate are shown in Figure 2.

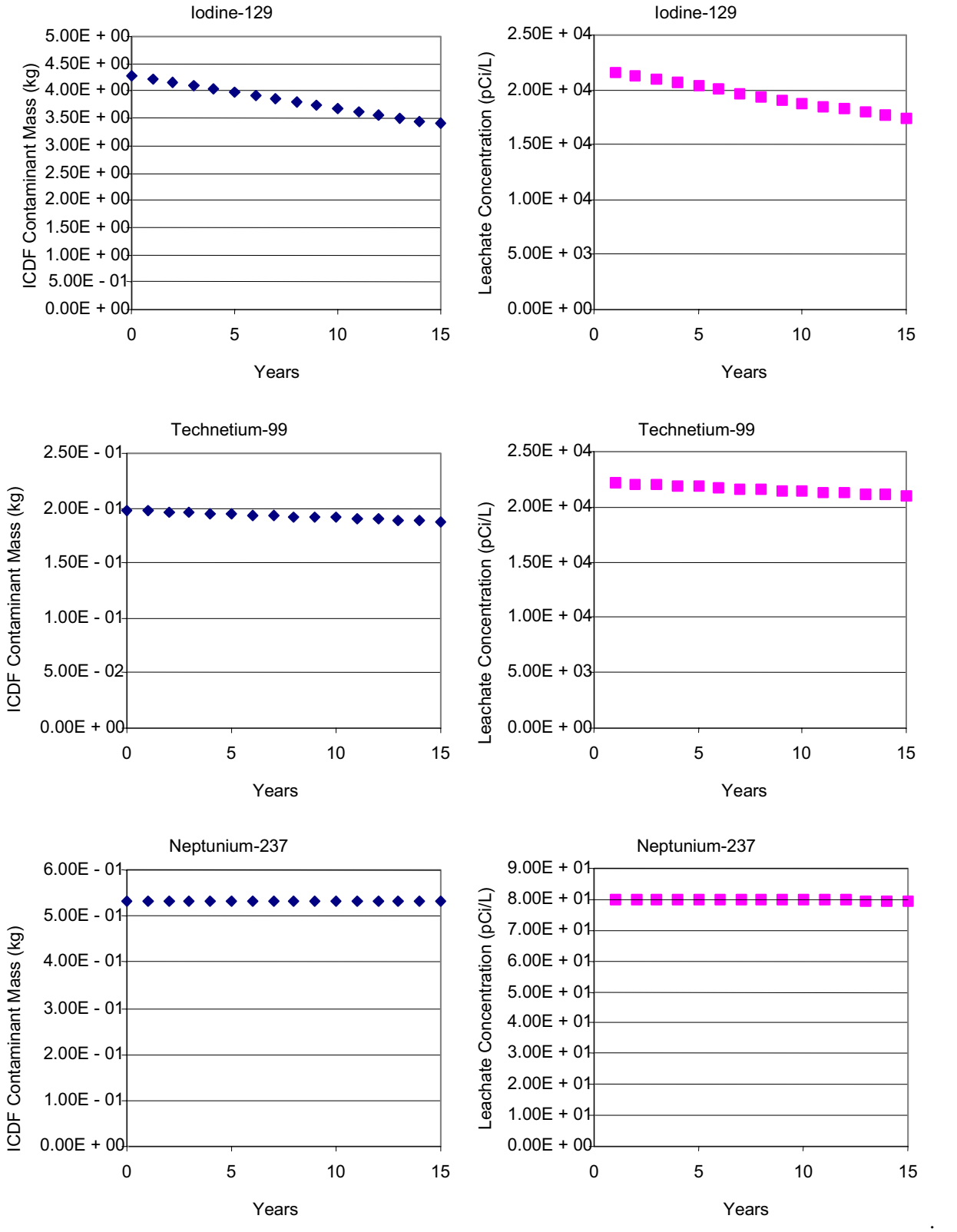

Figure 2. Evaluation of leachate concentration and residual mass in the ICDF at background recharge ratioed to 1.74 cm/yr recharge.

4. LEACHATE GENERATION AND CONTAMINANT REDUCTION DURING POST-CLOSURE PERIOD

An estimate of leachate generation and landfill contaminant migration in leachate during the 30-year post-closure period was performed using the same two-dimensional numerical code used to perform the landfill fate and transport modeling (i.e., STOMP). The simulation provides dilution/attenuation factors (DAF) for leachate that can be applied to design inventory constituents to determine estimated leachate concentration based on given landfill source concentrations. The simulation input parameters and overall physical conceptual model are described in detail in "Fate and Transport Modeling Results" (EDF-ER-275). To modify the model for assessment of the leachate generation, the top of the clay layer of the landfill liner was assumed to be a no-flow boundary to simulate the presence of the synthetic liner component. In addition, the sides of the operations layer immediately overlying the synthetic liner was assumed to be a seepage face, allowing leachate to exit the system when local hydraulic head exceeded atmospheric pressure.

A group of surrogates was selected to represent the entire list of contaminants of concern. Contaminants were assigned a surrogate only on the basis of relative mobility based on their distribution coefficients (K_d). For radioactive or environmentally decaying contaminants, the breakthrough curves of the appropriate surrogates were decayed individually. The methodology and results for the evaluation of leachate generation and constituent migration are presented below.

4.1 Leachate Generation Simulation

4.1.1 Introduction

The STOMP code was used to simulate leachate generation curves for the landfill. This model is intended to support decisions regarding leachate management and evaporation pond management during the post-closure period and to facilitate understanding of the mobility of contaminants within the facility. The approach and methodology used in this evaluation are described in the following sections.

4.1.2 Approach

This section describes the methods used to simulate the volume and contaminant concentrations of leachate collected during the 30-year post-closure period of the ICDF. During the post-closure period, the cap and the liner are assumed to remain intact and function as designed. The 60% design two-dimensional (vertical and horizontal parallel to groundwater flow) numerical model used to simulate the contaminant transport from the ICDF was amended to conduct the simulations. Hydraulic properties and ICDF construction parameters remained the same, with the exception that the top of the clay layer changed to a no-flow boundary to simulate the functioning synthetic liner. The side boundaries of the model remained no-flow, except immediately above the clay, where the boundary allowed flow and contaminants to exit the model domain when the local hydraulic pressure exceeded atmospheric pressure (seepage boundary). The flow exiting the model through these boundaries represented the leachate collected during the post-closure period.

4.1.3 Methodology

The modeling effort used the STOMP version 2.0 finite difference code developed by Pacific Northwest National Laboratory (PNNL) to conduct the simulations. A description of the STOMP code is found in the Theory Guide (PNNL-11217 1996) and the User's Guide (PNNL-12034 2000). Quantitative predictions of hydrogeologic flow and contaminant transport are generated from the numerical solution of

non-linear partial differential equations that describe subsurface environment flow and transport phenomena. STOMP capabilities include, among others, the simulation of saturated and unsaturated flow regimes, transport of radioactive elements and non-decaying contaminants, and transport of aqueous phase and non-aqueous phase organic compounds. A complete description of STOMP capabilities, the actual equations, and the partial differential approximations are contained within the Theory Guide and User's Guide and are not repeated here, except where necessary to describe input parameters.

The length dimension of the ICDF facility in the numerical model was determined from preliminary construction drawings (DOE-ID 2002) to be about 160 m. The side slope of the facility is ~3:1, so for the estimated waste volume (510,000 yd^3 or 389,923 m^3), the slope of the sides increases the area at the top of the waste by a factor of ~1.74:1. Therefore, the simulation of leachate accumulation increased by the specified design recharge rate (0.0001 m/yr) by a factor of 1.74. To account for the width of the facility, the leachate volume calculated to exit the model boundaries was multiplied by 194, which represented the width dimension determined from preliminary construction drawings (DOE-ID 2002). The concentration of the contaminants was assumed to remain uniform across the width of the facility.

4.1.3.1 Assumptions. The following assumptions were applied to support development of the leachate generation model:

1. The landfill was assumed to be filled to capacity at the start of the simulation (i.e., the design volume of waste soil is in place at time zero [T0], or the start of the simulation).

2. The initial waste soil moisture content is assumed to be at equilibrium with a steady state background recharge of 0.01 m/yr. It should be noted that while heavier precipitation events would be anticipated to produce larger quantities of leachate, precipitation pulses would tend to be attenuated or buffered to some degree by waste in the landfill.

3. The final landfill cover is assumed to be in place for the duration of the entire simulation, with net recharge to the landfill at the selected maximum design recharge rate of 0.0001 m/yr.

4. Contaminant mass leaves the landfill only by leachate transport and/or by decay (i.e., radioactive decay or environmental degradation), as applicable.

5. The synthetic high-density polyethylene (HDPE) liner component is assumed to be in place and to provide an impermeable layer at the top of the clay liner component for the duration of the simulation.

6. The lateral sides of the landfill model domain are assumed to be seepage boundaries that permit flow of leachate when local hydraulic pressure exceeds one atmosphere.

7. The simulation period is assumed to be limited to the 30-year post-closure period.

8. There are assumed to be no limits to solubility of the waste constituents simulated.

4.1.3.2 Computations. Simulating water and contaminant transport through the vadose zone requires the solution of the non-linear partial differential equations used to describe flow through unsaturated porous media. Solution of the equations requires moisture retention (aqueous phase pressure and moisture content) and fluid transport (hydraulic conductivity and moisture content or aqueous phase pressure) characteristic data for the porous media contained within the model domain. The model uses functional relationships (referred to as characteristic curves) to describe the characteristic data. The

equation used in the model was developed by van Genuchten to describe the moisture retention characteristic of the porous media:

$$S_w = \{1 + (\alpha[\frac{P_g - P_w}{\rho_w g}])^n\}^{-m} \quad for\ P_g - P_w > 0$$
$$S_w = 1 \quad for\ P_g - P_w \leq 0 \tag{5}$$

where

S_w = degree of water saturation of the porous media (dimensionless)

P_g = absolute pressure of the gas phase present (Pa, atmospheric pressure for these simulations)

P_w = absolute pressure of the water phase present (Pa)

ρ_w = density of water (kg/m^3)

g = acceleration of gravity (m/s^2)

α (1/m), n, and m are curve fit parameters, and m = 1 - 1/n except for basalt.

The Mualem equation was used to describe hydraulic conductivity as a function of moisture content:

$$k_{rw} = (S_w)^{1/2}\{1 - (1 - [S_w]^{1/m})^m\}^2 \quad and$$
$$K = k_{rw} * K_{sat} \tag{6}$$

where

K_{sat} = permeability (cm^2) or hydraulic conductivity (cm/s)

k_{rw} = relative permeability or hydraulic conductivity

K_{sat} = saturated permeability (cm^2) or saturated hydraulic conductivity (cm/s)

S_w and m are defined as before.

Table 3 presents the characteristic curve parameters of the different layers used in the leachate simulation, and Table 4 presents the hydraulic properties for the different layers. The saturated moisture content of each model layer type was assumed to equal the porosity. The surrogate distribution coefficients for the surrogates in the waste and operations layers are shown in Table 5.

Table 3. Summary of soil properties and moisture content-aqueous pressure relationship curve fit parameters.

Model Layer Type	Saturated Moisture Content	Residual Moisture Content	Curve Fit Parameter α (1/m)	Curve Fit Parameter n	Curve Fit Parameter m
Clay	Top of Clay is No-Flow Boundary				
Operations Layer	0.275	0.083	1.066	1.523	0.343
Waste	0.266	0.072	1.066	1.523	0.343

Table 4. Summary of soil hydraulic and contaminant transport properties.

Model Layer Type	Bulk Density (kg/m^3)	Saturated Hydraulic Conductivity (cm/s)	Longitudinal Dispersivity (m)	Transverse Dispersivity (m)
Clay	Top of Clay is No-Flow Boundary			
Operations Layer	1922	1E - 04	5	0
Waste	1946	1E - 03	5	0

Table 5. Contaminant distribution coefficients and weighted averages for the different surrogates and model layer types.

	Distribution Coefficient (K_d) (cm^3/g)							
Model Layer Type	Surrogate 1	Surrogate 2	Surrogate 3	Surrogate 4	Surrogate 5	Surrogate 6	Surrogate 7	Surrogate 8
Operations Layer	0	0	0.2	6	8	24	16	340
Waste	0	0	0.2	6	8	12	16	340

4.1.4 Simulation Output and Discussion

The results of the model indicate that no leachate accumulates after the cover is placed until the fourth year of the post-closure period.[b] The coincident arrival of the contaminants results from the fact that the transport tends to be dominated by drainage of initial moisture and diffusion at the design recharge rate. Also, the water must accumulate in the seepage boundary cells until the hydraulic pressure exceeds atmospheric pressure and the capillary pressure of the operations layer. The maximum simulated leachate generation rate is approximately 2.14E + 04 L/yr, and cumulative leachate volume for the simulation period is estimated at 4.23E + 05 liters (Figure 3). The more mobile contaminants may have arrived at the boundary cells sooner than the much less mobile contaminants, but transport across the seepage boundary did not occur until all the contaminants were present in the leachate. As indicated in Table 6, the leachate concentration of any contaminant less mobile than uranium is a small fraction of the waste soil concentration, and no significant percentage of any contaminant is collected in the leachate, even though the concentrations may be greatly elevated.

b. Note that the actual leachate flow is expected to transition from the operational period through the post-closure period.

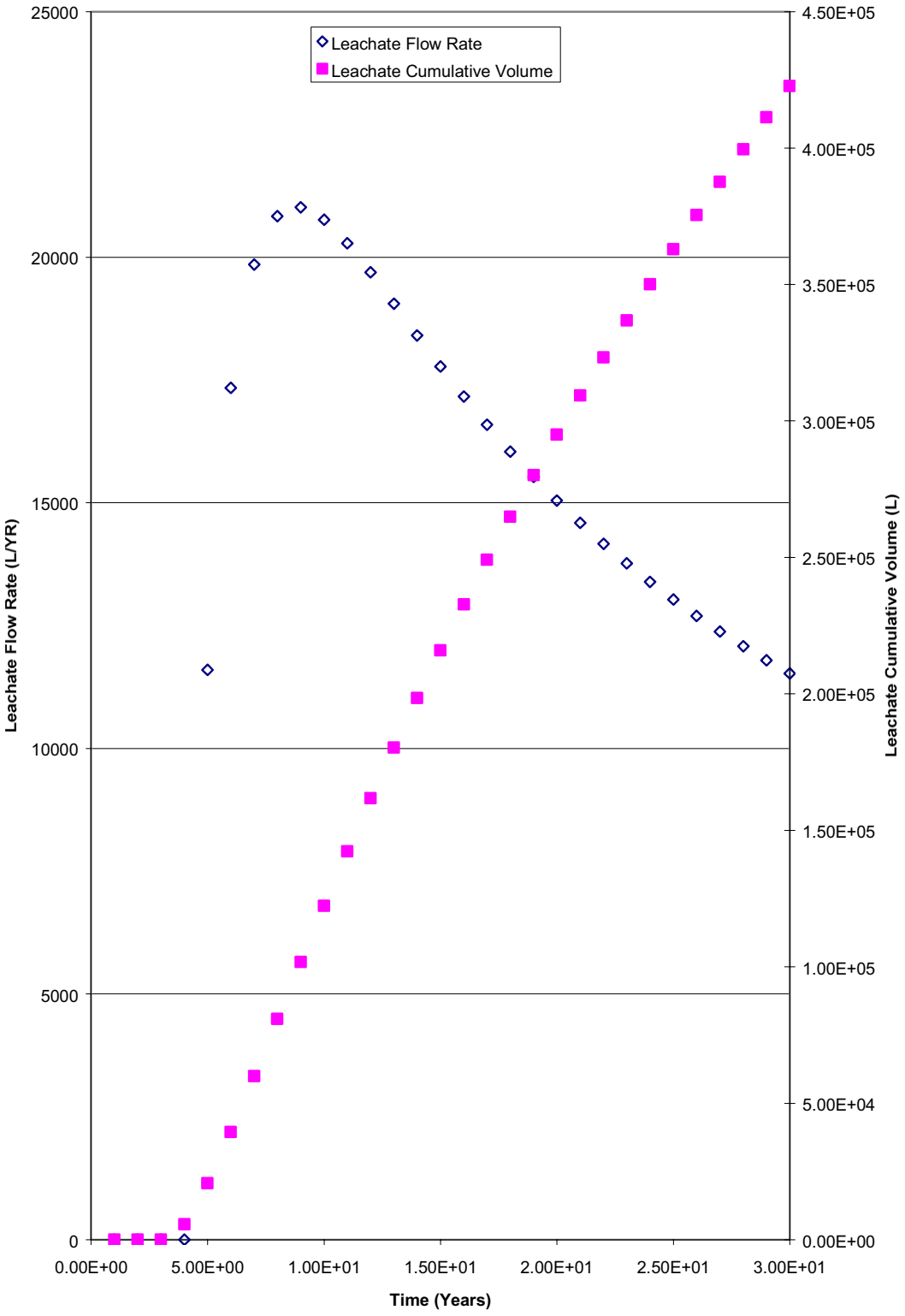

Figure 3. Leachate generation rate and cumulative leachate volume for the 30-year post-closure simulation period.

Table 6. Summary of Post-Closure Leachate Modeling Results at 0.0001 m/yr Recharge Rate.

	Half-Life (yr)	Design Inventory Concentration (mg/kg or pCi/kg)	Model Surrogate	Maximum Concentration (mg/L or pCi/L)	Average Concentration (mg/L or pCi/L)	Percentage of Inventory in Leachate
Radionuclides						
H-3	1.24E + 01	4.96E + 04	Surrogate 1	1.10E + 05	8.39E + 04	0.12%
I-129	1.57E + 07	1.30E + 03	Surrogate 2	7.36E + 03	5.80E + 03	0.32%
Tc-99	2.13E + 05	5.76E + 03	Surrogate 3	8.05E + 03	5.29E + 03	0.07%
U-234	2.45E + 05	6.03E + 03	Surrogate 4	4.22E + 00	1.57E + 00	0.00%
U-235	7.04E + 08	1.10E + 02	Surrogate 4	7.72E - 02	2.88E - 02	0.00%
U-236	2.34E + 07	2.02E + 02	Surrogate 4	1.42E - 01	5.28E - 02	0.00%
U-238	4.47E + 09	1.95E + 03	Surrogate 4	1.37E + 00	5.10E - 01	0.00%
Np-237	2.14E + 06	6.43E + 02	Surrogate 5	1.64E - 01	5.99E - 02	0.00%
Co-60	5.27E + 00	1.93E + 05	Surrogate 5	1.53E – 00	1.10E + 00	0.00%
Sr-90	2.91E + 01	2.29E + 07	Surrogate 6	6.52E + 02	2.74E + 02	0.00%
Pu-239	2.41E + 04	6.66E + 03	Surrogate 7	1.32E - 01	4.68E - 02	0.00%
Pu-240	6.54E + 03	1.50E + 03	Surrogate 7	2.97E - 02	1.05E - 02	0.00%
Cs-137	3.00E + 01	2.44E + 07	Surrogate 8	1.48E - 03	5.92E - 04	0.00%
Eu-155	4.96E + 00	1.76E + 05	Surrogate 8	5.09E - 07	3.65E - 07	0.00%
Organic						
Tributylphosphate	1.16E + 00	3.64E - 01	Surrogate 1	4.43E - 02	5.37E - 03	0.00%
2-Nitroaniline	NA	2.72E - 02	Surrogate 2	1.54E - 01	1.22E - 01	0.32%
Benzene	1.00E + 00	6.03E - 01	Surrogate 2	–5.01E – 02	–5.19E - 03	0.00%
Toluene	4.79E - 02	9.82E - 01	Surrogate 3	–7.97E - 27	–2.94E - 28	0.00%
Xylene (total)	5.12E - 01	3.45E + 00	Surrogate 3	–1.62E - 03	–1.02ED - 04	0.00%
Dibenzofuran	5.94E - 02	3.24E - 01	Surrogate 7	–8.90E - 29	–3.29E - 30	0.00%
Aroclor-1260	3.88E - 02	7.21E - 01	Surrogate 6	–1.69E - 44	–6.24E - 46	0.00%
Chrysene	3.76E + 00	2.65E - 01	Surrogate 8	3.73E - 13	2.46E - 13	0.00%
Inorganic						
Sulfate	NA	2.05E + 01	Surrogate 1	1.16E + 02	9.18E + 01	0.32%
Sulfide	NA	7.59E + 02	Surrogate 1	4.30E + 03	3.39E + 03	0.32%
Cyanide	NA	3.37E - 01	Surrogate 2	1.91E + 00	1.51E + 00	0.32%
Arsenic	NA	5.65E + 00	Surrogate 7	1.12E - 04	3.97E - 05	0.00%
Boron	NA	1.85E + 02	Surrogate 3	2.58E + 02	1.70E + 02	0.07%
Molybdenum	NA	1.02E + 01	Surrogate 5	2.59E - 03	9.48E - 04	0.00%
Cadmium	NA	3.59E + 00	Surrogate 4	–2.51E - 03	–9.37E – 04	0.00%
Cobalt	NA	6.04E + 00	Surrogate 5	–1.54E - 03	–5.62E - 04	0.00%
Aluminum	NA	7.08E + 03	Surrogate 7	1.40E - 01	4.97E - 02	0.00%
Lead	NA	5.76E + 01	Surrogate 7	1.14E - 03	4.05E - 04	0.00%
Zirconium	NA	6.91E + 01	Surrogate 8	8.39E - 09	2.88E - 09	0.00%

The leachate generation simulation can be extrapolated to all the constituents in the landfill design inventory by correlating the K_ds of the constituents in the design inventory to the K_ds of the simulated surrogates. As shown in the simulation results (Table 6), no significant quantity of the inventory of any

constituents similar to, or less mobile than, surrogate 4 are removed from the system in the post-closure period. Appendix D presents the simulated peak aqueous concentration for leachate during the post-closure period using a beginning inventory based on the facility design inventory.

5. CONCLUSIONS

Concentrations of design inventory constituents in ICDF landfill leachate were simulated over the 15-year operations period and an assumed 30-year post-closure period. The purpose of the study was to examine the change in landfill contaminant mass and leachate concentration over time. As long as the landfill is generating leachate, it will be managed in a manner that is protective of human health and the environment, and in accordance with all ARARS.

The conclusions of each evaluation include the following:

- Geochemical Modeling
  - Detailed discussion of results are found in Section 2.3 with output provided in Appendix B.
  - Leachate is a brackish water (total dissolved solids around 46,000 mg/L) dominated by sodium and sulfate with a pH of 8.0.
  - The water chemistry is most influenced by the oxidation of sulfide minerals, equilibration of carbonates, and dissolution of the more plentiful of the soluble components of the design inventory.
  - Elements that were only slightly soluble include barium, zinc, plutonium, and uranium.
  - Salts of most anionic constituents were completely dissolved before equilibration could be reached.
- Leachate Generation During Operations
  - Detailed discussion of results are found in Section 3.1.4 with output provided in Appendix C.
  - Contaminant mass reduction due to leaching of selected highly mobile contaminants is typically around 20% of the design inventory mass over the 15-year simulation period.
  - Technitium-99 has a K_d value of 0.2 ml/g and experienced a contaminant reduction of approximately 5%.
  - Uranium isotopes and neptunium-237 have K_d values of 6.0 and 8.0 ml/g, respectively, and experienced a contaminant reduction of less than 1%.
- Leachate Generation During Post-Closure
  - Detailed discussion of results are found in Section 4.1.4 with output provided in Appendix D.
  - Less than 1% of the inventory masses of the most mobile constituents may be removed in leachate during that time period.

- The decrease in contaminant mass leached is primarily due to the expected substantial reduction in leachate generation provided by the effective function of the final landfill cover system.

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Appendix A

Constituent Solubility Modeled Using PHREEQC

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Table A-1. Constituents considered significantly leachable (Kd <20).

Constituent	Kd (L/kg)	Reference
1,1,1-Trichloroethane	0.41	1
1,1,2,2-Tetrachloroethane	0.24	1
1,1,2-Trichloroethane	0.23	1
1,1-Dichloroethane	0.16	1
1,1-Dichloroethene	0.20	1
1,2,4-Trichlorobenzene	4.98	1
1,2-Dichlorobenzene	1.14	1
1,2-Dichloroethane	0.11	1
1,2-Dichloroethene (total)	0.11	1
1,3-Dichlorobenzene	4.44	2
1,4-Dichlorobenzene	1.85	1
1,4-Dioxane	0.00	2
2,4,5-Trichlorophenol	2.12	2
2,4,6-Trichlorophenol	7.54	2
2,4-Dichlorophenol	1.04	2
2,4-Dimethylphenol	0.63	1
2,4-Dinitrophenol	0.06	2
2,4-Dinitrotoluene	0.29	1
2,6-Dinitrotoluene	0.21	1
2-Butanone	0.04	2
2-Chlorophenol	0.26	2
2-Hexanone	0.04	2
2-Methylnaphthalene	unknown	none
2-Methylphenol	0.27	1
2-Nitroaniline	0.05	2
2-Nitrophenol	0.13	2
3,3'-Dichlorobenzidine	1.94	2
3-Methyl Butanal	unknown	none
3-Nitroaniline	0.04	2
4,6-Dinitro-2-methylphenol	unknown	none
4-Chloro-3-methylphenol	2.33	2
4-Chloroaniline	0.13	2
4-Methyl-2-Pentanone	unknown	none
4-Methylphenol	0.02	2
4-Nitroaniline	unknown	none
4-Nitrophenol	0.15	2
Acenaphthene	14.69	1

Table A-1. (continued).

Constituent	Kd (L/kg)	Reference
Acetone	0.00	1
Acetonitrile	0.00	2
Acrolein	0.00	2
Acrylonitrile	0.00	2
Aramite	unknown	none
As	3.00	1
At	0.00	1
B	5.00	1
Benzene	0.19	1
Benzidine	0.04	2
Benzoic acid	0.14	2
bis(2-Chloroethoxy)methane	0.01	2
bis(2-Chloroethyl)ether	0.23	1
bis(2-Chloroisopropyl)ether	0.70	2
bis(2-Ethylhexyl)phthalate	18.00	1
Butane,1,1,3,4-Tetrachloro-	unknown	none
C-14	5.00	1
Ca	5.00	1
Carbazole	10.17	1
Carbon Disulfide	0.14	1
Cd	6.00	1
Chlorobenzene	0.67	1
Chloroethane	0.05	2
Chloromethane	0.02	2
Cl	0.00	1
Co	10.00	1
Cu	20.00	1
Cyanide	0.00	1
Decane, 3,4-Dimethyl	unknown	none
Diacetone alcohol	unknown	none
Dibenzofuran	unknown	none
Diethylphthalate	0.25	1
Dimethyl Disulfide	0.11	2
Dimethylphthalate	0.07	2
Di-n-butylphthalate	4.70	1
Eicosane	unknown	none
Ethyl cyanide	unknown	none
Ethylbenzene	0.61	1

Table A-1. (continued).

Constituent	Kd (L/kg)	Reference
Famphur	unknown	none
Fluoride	0.00	1
Heptadecane, 2,6,10,15-Tetra	unknown	none
Hexachlorobutadiene	10.17	2
Hexachloroethane	5.34	1
I	0.00	1
Isobutyl alcohol	unknown	none
Isophorone	0.14	1
Isopropyl Alcohol/2-propanol	unknown	none
K	15.00	1
Kepone	unknown	none
Kr	0.00	1
Mesityl oxide	unknown	none
Methyl Acetate	0.00	2
Methylene Chloride	0.03	1
Mg	5.00	1
Mo	10.00	1
Naphthalene	3.57	1
Nitrate	0.00	1
Nitrate/Nitrite-N	0.00	1
Nitrite	0.00	1
Nitrobenzene	0.36	1
N-Nitroso-di-n-propylamine	0.07	1
N-Nitrosodiphenylamine	3.87	1
Np	8.00	1
Octane,2,3,7-Trimethyl	unknown	none
o-Toluenesulfonamide	unknown	none
P	5.00	1
Phenol	0.09	1
Phenol,2,6-Bis(1,1-Dimethyl)	unknown	none
p-Toluenesulfonamide	unknown	none
Rn	0.00	1
Se	4.00	1
Styrene	2.74	1
Sulfate	14.00	1
Sulfide	14.00	1
Tc	0.20	1
Tetrachloroethene	0.80	1

Table A-1. (continued).

Constituent	Kd (L/kg)	Reference
Toluene	1.00	1
Tributylphosphate	unknown	none
Trichloroethene	0.28	1
Tritium	0.00	1
U	6.00	1
Undecane,4,6-Dimethyl-	unknown	none
V	6.00	1
Xe	0.00	1
Xylene (ortho)	0.72	1
Xylene (total)	0.59	1
Zn	16.00	1

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Table A-2. Constituents not considered significantly leachable (Kd>20 L/kg).

Constituent	Kd (L/kg)	Reference
2-Chloronaphthalene	2.44E+01	2
4-Bromophenyl-phenylether	3.52E+01	2
4-Chlorophenyl-phenylether	2.22E+01	2
Ac	4.50E+02	1
Acenaphthylene	2.17E+01	2
Ag	9.00E+01	1
Al	2.50E+02	1
Am	3.40E+02	1
Anthracene	7.05E+01	1
Aroclor-1016	1.00E+02	1
Aroclor-1254	1.00E+02	1
Aroclor-1260	1.00E+02	1
Aroclor-1268	1.00E+02	1
Ba	5.00E+01	1
Be	2.50E+02	1
Benzo(a)anthracene	1.07E+03	1
Benzo(a)pyrene	1.20E+03	1
Benzo(b)fluoranthene	3.69E+03	1
Benzo(g,h,i)perylene	3.14E+04	2
Benzo(k)fluoranthene	3.69E+03	1
Bi	1.00E+02	1
Bk	4.00E+03	1
Butylbenzylphthalate	4.12E+01	1
Ce	5.00E+02	1
Cf	5.10E+02	1
Chrysene	1.19E+03	1
Cm	4.00E+03	1
Cr	3.00E+01	1
Cs	5.00E+02	1
Dibenz(a,h)anthracene	5.37E+03	1
Di-n-octylphthalate	2.50E+05	1
Dysprosium	2.40E+02	1
Er	2.40E+02	1
Eu	2.40E+02	1
Fe	2.20E+02	1
Fluoranthene	1.47E+02	1
Fluorene	2.31E+01	1

Table A-2. (continued).

Constituent	Kd (L/kg)	Reference
Fr	5.00E+02	1
Gd	2.40E+02	1
Hexachlorobenzene	2.40E+02	1
Hexachlorocyclopentadiene	6.00E+02	1
Hf	4.50E+02	1
Hg	1.00E+02	1
Ho	2.50E+02	1
In	3.90E+02	1
Indeno(1,2,3-cd)pyrene	1.04E+04	1
La	1.20E+03	1
Mn	5.00E+01	1
Na	7.60E+01	1
Nb	1.60E+02	1
Nd	2.40E+02	1
Ni	1.00E+02	1
Pa	5.50E+02	1
Pb	1.00E+02	1
Pd	5.50E+01	1
Pentachlorophenol	2.38E+03	2
Phenanthrene	1.89E+02	2
Pm	2.40E+02	1
Po	1.50E+02	1
Pr	2.40E+02	1
Pu	1.40E+02	1
Pyrene	2.04E+02	1
Ra	1.00E+02	1
Rb	5.50E+01	1
Ru	5.50E+01	1
Sb	5.00E+01	1
Sc	3.10E+02	1
Sm	2.45E+02	1
Sn	1.30E+02	1
Sr	2.40E+01	1
Ta	2.20E+02	1
Tb	2.40E+02	1
Te	1.25E+02	1
Th	1.00E+02	1
Tl	1.00E+02	1

Table A-2. (continued).

Constituent	Kd (L/kg)	Reference
Tm	2.40E+02	1
Y	1.70E+02	1
Zr	6.00E+02	1

References:

1. Jenkins, T., DOE, letter to Martin Doornbos, BBWI, July 3, 2001, *Kd values for INTEC groundwater modeling* (EM-ER-01-115).
2. Verschueren, Karel, 1983, Handbook of Environmental Data on Organic Chemicals, Second Edition, Van Nostrand Reinhold pub. New York, New York, and Callahan, et.al, 1979 Water-Related Environmental Fate of 123 Priority Pollutants, EPA-440/4-79-029 a and b.

Table A-3. Screened constituents used in geochemical modeling.

Cations	Element	Symbol	Element Quantity from Design Inventory (kg)	Percent of Total Design Inventory Mass (a)
	Calcium	Ca	1.24E+07	2.12E+00
	Iron	Fe	6.00E+06	1.03E+00
	Aluminum	Al	4.16E+06	7.11E-01
	Magnesium	Mg	2.62E+06	4.48E-01
	Potassium	K	6.73E+05	1.15E-01
	Terbium	Tb	3.35E+05	5.73E-02
	Sodium	Na	1.25E+05	2.14E-02
	Zinc	Zn	1.22E+05	2.08E-02
	Manganese	Mn	1.21E+05	2.06E-02
	Ytterbium	Yb	1.14E+05	1.95E-02
	Barium	Ba	1.06E+05	1.80E-02
Anions (b)	Carbon (rad)	C	4.90E-09	N/A (c)
	Iodine (rad)	I	4.30E+00	N/A (c)
	Technitium (rad)	Tc	1.99E-01	N/A (c)
	Tellurium (rad)	Te	1.13E-08	N/A (c)
	Plutonium (rad)	Pu	7.50E-02	N/A (c)
	Uranium (rad)	U	3.47E+03	N/A (c)
	Phosphorus	P	5.70E+04	N/A (c)
	Vanadium	V	1.26E+04	N/A (c)
	Sulfate	SO4	1.20E+04	N/A (c)
	Arsenic	As	3.33E+03	N/A (c)
	Nitrate	NO3	2.30E+03	N/A (c)
	Fluoride	F	2.26E+03	N/A (c)
	Chloride	Cl	1.09E+03	N/A (c)
	Selenium	Se	4.99E+02	N/A (c)
	Cyanide	CN	1.97E+02	N/A (c)
	Nitrite	NO2	4.97E+00	N/A (c)
	Boron	B	1.08E+05	N/A (c)
	Sulfide	S	4.44E+05	N/A (c)

Notes;
(a). Calculated by dividing the kg of each constituent by 5.85E+08 kg, the total inventory mass.
(b). Radioactive anions expressed as total mass of all reported isotopes.
(c). Anions were not screened on the basis of percentage of total inventory.mass.

Table A-4. Organic and cationic constituents eliminated during screening process[a].

Organics	Constituent	kg	% of total
	1,1,1-Trichloroethane	7.43E+00	1.27E-06
	1,1,2,2-Tetrachloroethane	2.34E-02	4.01E-09
	1,1,2-Trichloroethane	1.15E-01	1.96E-08
	1,1-Dichloroethane	1.11E+00	1.89E-07
	1,1-Dichloroethene	7.01E-01	1.20E-07
	1,2,4-Trichlorobenzene	5.39E+00	9.21E-07
	1,2-Dichlorobenzene	5.39E+00	9.21E-07
	1,2-Dichloroethane	2.55E-03	4.36E-10
	1,2-Dichloroethene (total)	1.54E-01	2.62E-08
	1,3-Dichlorobenzene	5.39E+00	9.21E-07
	1,4-Dichlorobenzene	2.13E+02	3.64E-05
	1,4-Dioxane	8.91E-03	1.52E-09
	2,4,5-Trichlorophenol	2.11E+01	3.61E-06
	2,4,6-Trichlorophenol	8.65E+00	1.48E-06
	2,4-Dichlorophenol	1.02E+01	1.75E-06
	2,4-Dimethylphenol	8.65E+00	1.48E-06
	2,4-Dinitrophenol	2.41E+01	4.12E-06
	2,4-Dinitrotoluene	5.39E+00	9.21E-07
	2,6-Dinitrotoluene	9.80E+00	1.67E-06
	2-Butanone	1.17E+01	2.00E-06
	2-Chloronaphthalene	5.39E+00	9.21E-07
	2-Chlorophenol	8.65E+00	1.48E-06
	2-Hexanone	1.28E+00	2.18E-07
	2-Methylnaphthalene	2.42E+02	4.14E-05
	2-Methylphenol	9.78E+00	1.67E-06
	2-Nitroaniline	1.29E+01	2.20E-06
	2-Nitrophenol	8.65E+00	1.48E-06
	3,3'-Dichlorobenzidine	5.39E+00	9.21E-07
	3-Methyl Butanal	1.06E-01	1.81E-08
	3-Nitroaniline	1.29E+01	2.20E-06
	4,6-Dinitro-2-methylphenol	2.11E+01	3.61E-06
	4-Bromophenyl-phenylether	5.39E+00	9.21E-07
	4-Chloro-3-methylphenol	8.65E+00	1.48E-06
	4-Chloroaniline	1.93E+01	3.30E-06
	4-Chlorophenyl-phenylether	5.39E+00	9.21E-07
	4-Methyl-2-Pentanone	1.40E+01	2.40E-06
	4-Methylphenol	1.83E+01	3.12E-06
	4-Nitroaniline	1.29E+01	2.20E-06
	4-Nitrophenol	2.44E+01	4.17E-06
	Acenaphthene	9.58E+01	1.64E-05
	Acenaphthylene	9.80E+00	1.67E-06
	Acetone	2.94E+02	5.02E-05
	Acetonitrile	8.91E-03	1.52E-09
	Acrolein	4.29E-03	7.33E-10

Table A-4. (continued).

Organics	Constituent	kg	% of total
	Acrylonitrile	4.29E-03	7.33E-10
	Anthracene	1.52E+02	2.59E-05
	Aramite	5.42E-02	9.27E-09
	Aroclor-1016	3.64E+00	6.22E-07
	Aroclor-1254	6.08E+01	1.04E-05
	Aroclor-1260	3.41E+02	5.84E-05
	Aroclor-1268	2.94E+01	5.03E-06
	Benzene	2.86E+02	4.89E-05
	Benzidine	1.38E-01	2.35E-08
	Benzo(a)anthracene	1.20E+02	2.05E-05
	Benzo(a)pyrene	4.97E+01	8.49E-06
	Benzo(b)fluoranthene	8.50E+01	1.45E-05
	Benzo(g,h,i)perylene	5.39E+00	9.21E-07
	Benzo(k)fluoranthene	8.81E+00	1.51E-06
	Benzoic acid	4.05E+00	6.93E-07
	bis(2-Chloroethoxy)methane	5.39E+00	9.21E-07
	bis(2-Chloroethyl)ether	5.39E+00	9.21E-07
	bis(2-Chloroisopropyl)ether	5.39E+00	9.21E-07
	bis(2-Ethylhexyl)phthalate	6.97E+01	1.19E-05
	Butane,1,1,3,4-Tetrachloro-	3.74E+00	6.39E-07
	Butylbenzylphthalate	3.22E+01	5.50E-06
	Carbazole	1.53E+01	2.62E-06
	Carbon Disulfide	2.16E+01	3.69E-06
	Chlorobenzene	3.11E+00	5.32E-07
	Chloroethane	1.43E-03	2.44E-10
	Chloromethane	1.67E-01	2.86E-08
	Chrysene	1.26E+02	2.15E-05
	Decane, 3,4-Dimethyl	7.64E-02	1.31E-08
	Diacetone alcohol	2.05E+03	3.50E-04
	Dibenz(a,h)anthracene	5.39E+00	9.21E-07
	Dibenzofuran	1.54E+02	2.62E-05
	Diethylphthalate	5.39E+00	9.22E-07
	Dimethyl Disulfide	1.40E+00	2.40E-07
	Dimethylphthalate	5.39E+00	9.21E-07
	Di-n-butylphthalate	1.13E+01	1.93E-06
	Di-n-octylphthalate	1.24E+01	2.12E-06
	Eicosane	1.34E+00	2.29E-07
	Ethyl cyanide	8.91E-03	1.52E-09
	Ethylbenzene	3.70E+01	6.32E-06
	Famphur	2.75E-02	4.71E-09
	Fluoranthene	3.61E+02	6.17E-05
	Fluorene	8.70E+01	1.49E-05
	Heptadecane, 2,6,10,15-Tetra	1.63E+00	2.78E-07
	Hexachlorobenzene	5.39E+00	9.21E-07
	Hexachlorobutadiene	9.80E+00	1.67E-06

Table A-4. (continued).

Organics	Constituent	kg	% of total
	Hexachlorocyclopentadiene	5.39E+00	9.21E-07
	Hexachloroethane	5.39E+00	9.21E-07
	Indeno(1,2,3-cd)pyrene	5.39E+00	9.21E-07
	Isobutyl alcohol	8.91E-03	1.52E-09
	Isophorone	5.39E+00	9.22E-07
	Isopropyl Alcohol/2-propanol	1.01E+00	1.72E-07
	Kepone	4.70E+01	8.03E-06
	Mesityl oxide	4.01E+01	6.86E-06
	Methyl Acetate	2.29E-01	3.92E-08
	Methylene Chloride	3.96E+01	6.77E-06
	Naphthalene	2.01E+02	3.44E-05
	Nitrobenzene	5.39E+00	9.21E-07
	N-Nitroso-di-n-propylamine	5.39E+00	9.21E-07
	N-Nitrosodiphenylamine	5.39E+00	9.21E-07
	Octane,2,3,7-Trimethyl	7.64E-02	1.31E-08
	o-Toluenesulfonamide	2.40E+00	4.09E-07
	Pentachlorophenol	2.65E+01	4.53E-06
	Phenanthrene	5.53E+02	9.46E-05
	Phenol	3.78E+01	6.46E-06
	Phenol,2,6-Bis(1,1-Dimethyl)	1.92E+00	3.28E-07
	p-Toluenesulfonamide	2.40E+00	4.09E-07
	Pyrene	1.20E+02	2.05E-05
	Styrene	4.86E-04	8.30E-11
	Tetrachloroethene	4.56E+00	7.80E-07
	Toluene	4.65E+02	7.95E-05
	Tributylphosphate	1.72E+02	2.94E-05
	Trichloroethene	3.41E+01	5.83E-06
	Undecane,4,6-Dimethyl-	7.64E-02	1.31E-08
	Xylene (ortho)	1.84E+00	3.14E-07
	Xylene (total)	1.64E+03	2.80E-04
Cations		kg	% of total
	Antimony	3.41E+03	5.83E-04
	Arsenic	3.33E+03	5.69E-04
	Beryllium	1.70E+02	2.90E-05
	Cadmium	2.11E+03	3.60E-04
	Chloride	1.09E+03	1.87E-04
	Chromium	2.41E+04	4.13E-03
	Cobalt	3.53E+03	6.03E-04
	Copper	1.75E+04	2.99E-03
	Cyanide	1.97E+02	3.37E-05
	Dysprosium	3.47E+04	5.93E-03
	Fluoride	2.26E+03	3.87E-04
	Lead	3.38E+04	5.77E-03
	Mercury	5.53E+03	9.45E-04
	Molybdenum	5.95E+03	1.02E-03

Table A-4. (continued).

Organics	Constituent	kg	% of total
	Nickel	1.15E+04	1.97E-03
	Nitrate	2.30E+03	3.93E-04
	Nitrate/Nitrite-N	1.30E+02	2.22E-05
	Nitrite	4.97E+00	8.49E-07
	Phosphorus	5.70E+04	9.74E-03
	Selenium	4.99E+02	8.52E-05
	Silver	5.75E+03	9.84E-04
	Strontium	1.06E+04	1.82E-03
	Sulfate	1.20E+04	2.05E-03
	Thallium	2.17E+02	3.70E-05
	Vanadium	1.26E+04	2.15E-03
	Zirconium	4.04E+04	6.91E-03

a. Criterion for organics to be included was a mass concentration greater than 1% of total waste mass; criterion for cations to be included was a mass concentration greater than 0.01% of total waste mass; Total waste mass assumed to be 5.85E+08 kg.

Table A-5. Quantities of mineral phases used in geochemical modeling constituent.[a]

Constituent [a]	Chemical Formula	Constituent Molar Mass (g/mol)	Mass Concentration from Design Inventory (mg/kg)[b]	Moles of Constituent per (kg)	Mineral Source(s)	Moles of Mineral Sources Exposed to 1L Leachate[c]	Mineral(s) Controlling Solubility
Aluminum	Al	27.0	7.11E+03	2.64E-01	Albite (NaAlSi3O8), Orthoclase (KAlSi3O8), Illite (K0.6Mg0.25Al2.3Si3.5O10(OH)2)	14, 7.8, 4.1[d]	Kaolinite (Al2Si2O5(OH)4)
Arsenic	As	74.9	5.69E+00	7.59E-05	Ca3(AsO4)2	6E-04	none
Barium	Ba	137.0	1.80E+02	1.32E-03	Barite (BaSO4)	2E-02	Barite (BaSO4)
Boron	B	10.8	1.85E+02	1.71E-02	Borax (Na2B4O5(OH)4.8H2O)	7E-02	Borax (Na2B4O5(OH)4.8H2O)
Calcium	Ca	40.0	2.12E+04	5.30E-01	Calcite (CaCO3)	6.1[d]	Calcite (CaCO3)
Carbon (rad)	C	14.0	1.03E-11	7.39E-16	not considered[e]	not considered[e]	not considered[e]
Chloride	Cl	35.5	1.87E+00	5.26E-05	Halite (NaCl)	9E-04	none
Cyanide	CN	26.0	3.37E-01	1.29E-05	NaCN	2.16E-04	oxidized to NO3
Fluoride	F	19.0	3.87E+00	2.03E-04	Fluoroapatite (Ca5(PO4)3F)	3E-03	Fluoroapatite (Ca5(PO4)3F)
Iodine (rad)	I	129.0	7.35E-03	5.70E-08	NaI	9.49E-07	none
Iron	Fe	55.8	1.03E+04	1.84E-01	Fe(OH)3, pyrite (FeS2)	2.9, 0.17	Fe(OH)3
Magnesium	Mg	24.3	4.48E+03	1.84E-01	Enstatite (MgSiO3), Illite (K0.6Mg0.25Al2.3Si3.5O10(OH)2)	22, 4.1[d]	dolomite
Manganese	Mn	54.9	2.06E+02	3.76E-03	Birnessite (Mn8O14.5H2O)	8E-03	Birnessite (Mn8O14.5H2O)
Nitrate	NO3	62.0	3.93E+00	6.33E-05	Niter (KNO3)	1E-03	none
Nitrite	NO2	46.0	8.49E-03	1.84E-07	not considered[f]	not considered[f]	oxidized to NO3
Phosphorus	P	31.0	9.74E+01	3.14E-03	Fluoroapatite (Ca5(PO4)3F)	2E-02	Fluoroapatite (Ca5(PO4)3F)
Plutonium (rad)	Pu	244.0	1.28E-04	5.26E-10	PuO2	8.76E-09	PuO2
Potassium	K	39.1	1.15E+03	2.94E-02	Orthoclase (KAlSi3O8), Illite (K0.6Mg0.25Al2.3Si3.5O10(OH)2)	7.8, 4.1[d]	none
Selenium	Se	79.0	8.52E-01	1.08E-05	CaSeO4	6.7E-05	none
Sodium	Na	23.0	2.14E+02	9.31E-03	Albite (NaAlSi3O8), Halite (NaCl), NaI, NaCN	14 (4), 9E-04, 9.49E-07, 2.16E-04	none

Table A-5. (continued).

Constituent [a]	Chemical Formula	Constituent Molar Mass (g/mol)	Mass Concentration from Design Inventory (mg/kg)[b]	Moles of Constituent per (kg)	Mineral Source(s)	Moles of Mineral Sources Exposed to 1L Leachate[c]	Mineral(s) Controlling Solubility
Sulfate	SO4	96.0	2.05E+01	2.14E-04	Gypsum (CaSO4.2H2O), Barite (BaSO4)	0.0036, 0.022	none
Sulfide	S	32.1	7.59E+02	2.36E-02	Pyrite (FeS2), Sphalerite (ZnS)	0.34, 0.053	oxidized to SO4
Technitium (rad)	Tc	98.9	3.40E-04	3.43E-09	TcO2.2H20(amorphous)	5.72E-08	none
Tellurium (rad)	Te	128.0	2.38E-11	1.86E-16	not considered[g]	not considered[g]	not considered[g]
Terbium	Tb	158.9	5.73E+02	3.61E-03	Tb2O3	3E-02	none
Uranium (rad)	U	238.0	5.94E+00	2.49E-05	CaUO4	4.16E-04	CaUO4
Vanadium	V	50.9	2.15E+01	4.22E-04	Ca2V2O7	3.5E-03	Ca2V2O7
Ytterbium	Yb	173.0	1.95E+02	1.13E-03	Yb2O3	9.4E-03	Yb(OH)3
Zinc	Zn	65.4	2.08E+02	3.18E-03	Sphalerite (ZnS)	5E-02	Zincite (ZnCO3)

a. Radioactive constituents expressed as total mass of all reported isotopes

b. Calculated by dividing the kg of each constituent by 5.85E+08 kg, the total inventory mass.

c. Calculated by multiplying the moles/kg value by 16.7 (the number of kg soil exposed to 1L of leachate) and dividing by constituent's stochiometry in the mineral. Input into PHREEQC.

d. Moles of these minerals were derived from observed mineral abundance and not from design inventory (see text)

e. Radioactive carbon could not be considered separately from non-radioactive carbon, and was assumed to be completely soluble

f. Nitrite was not considered stable in soil, and was not considered in the analysis

g. No solubility data was found for tellurium, so it was assumed to be completely soluble

Table A-6. Organic Compounds from design inventory calculated mg/L assuming complete dissolution.

Constituent	Total (kg)	5.8504E+08 (mg/kg)	0.0638 (mg/L)
1,1,1-Trichloroethane	9.175492298	1.5684E-02	2.4583E-01
1,1,2,2-Tetrachloroethane	0.028938608	4.9465E-05	7.7531E-04
1,1,2-Trichloroethane	0.141619589	2.4207E-04	3.7942E-03
1,1-Dichloroethane	1.368989357	2.3400E-03	3.6677E-02
1,1-Dichloroethene	0.865453042	1.4793E-03	2.3187E-02
1,2,4-Trichlorobenzene	6.655879888	1.1377E-02	1.7832E-01
1,2-Dichlorobenzene	6.655879888	1.1377E-02	1.7832E-01
1,2-Dichloroethane	0.003147102	5.3793E-06	8.4316E-05
1,2-Dichloroethene (total)	0.189636546	3.2415E-04	5.0806E-03
1,3-Dichlorobenzene	6.655879888	1.1377E-02	1.7832E-01
1,4-Dichlorobenzene	263.2739454	4.5001E-01	7.0535E+00
1,4-Dioxane	0.010999277	1.8801E-05	2.9469E-04
2,4,5-Trichlorophenol	26.0930445	4.4601E-02	6.9907E-01
2,4,6-Trichlorophenol	10.67926988	1.8254E-02	2.8611E-01
2,4-Dichlorophenol	12.63537363	2.1598E-02	3.3852E-01
2,4-Dimethylphenol	10.67926988	1.8254E-02	2.8611E-01
2,4-Dinitrophenol	29.79645552	5.0931E-02	7.9829E-01
2,4-Dinitrotoluene	6.655879888	1.1377E-02	1.7832E-01
2,6-Dinitrotoluene	12.09928988	2.0681E-02	3.2416E-01
2-Butanone	14.45966536	2.4716E-02	3.8740E-01
2-Chloronaphthalene	6.655879888	1.1377E-02	1.7832E-01
2-Chlorophenol	10.67926988	1.8254E-02	2.8611E-01
2-Hexanone	1.577610208	2.6966E-03	4.2267E-02
2-Methylnaphthalene	299.4425884	5.1184E-01	8.0225E+00
2-Methylphenol	12.07213869	2.0635E-02	3.2343E-01
2-Nitroaniline	15.91623451	2.7206E-02	4.2642E-01
2-Nitrophenol	10.67926988	1.8254E-02	2.8611E-01
3,3'-Dichlorobenzidine	6.655879888	1.1377E-02	1.7832E-01
3-Methyl Butanal	0.130604732	2.2324E-04	3.4991E-03
3-Nitroaniline	15.91623451	2.7206E-02	4.2642E-01
4,6-Dinitro-2-methylphenol	26.0930445	4.4601E-02	6.9907E-01
4-Bromophenyl-phenylether	6.655879888	1.1377E-02	1.7832E-01
4-Chloro-3-methylphenol	10.67926988	1.8254E-02	2.8611E-01
4-Chloroaniline	23.86523056	4.0793E-02	6.3939E-01
4-Chlorophenyl-phenylether	6.655879888	1.1377E-02	1.7832E-01
4-Methyl-2-Pentanone	17.33648341	2.9633E-02	4.6447E-01
4-Methylphenol	22.56936671	3.8578E-02	6.0467E-01
4-Nitroaniline	15.91623451	2.7206E-02	4.2642E-01
4-Nitrophenol	30.1607092	5.1554E-02	8.0805E-01
Acenaphthene	118.3160089	2.0224E-01	3.1699E+00
Acenaphthylene	12.09928988	2.0681E-02	3.2416E-01
Acetone	362.9988875	6.2047E-01	9.7253E+00
Acetonitrile	0.010999277	1.8801E-05	2.9469E-04
Acrolein	0.005299652	9.0587E-06	1.4199E-04
Acrylonitrile	0.005299652	9.0587E-06	1.4199E-04
Anthracene	187.3670094	3.2027E-01	5.0198E+00
Aramite	0.066995597	1.1452E-04	1.7949E-03
Aroclor-1016	4.496729992	7.6863E-03	1.2047E-01

Table A-6. (continued).

Constituent	Total (kg)	5.8504E+08 (mg/kg)	0.0638 (mg/L)
Aroclor-1254	75.10023766	1.2837E-01	2.0120E+00
Aroclor-1260	421.5951954	7.2063E-01	1.1295E+01
Aroclor-1268	36.36971761	6.2167E-02	9.7440E-01
Benzene	352.9562773	6.0331E-01	9.4562E+00
Benzidine	0.169988829	2.9056E-04	4.5543E-03
Benzo(a)anthracene	148.0297692	2.5303E-01	3.9659E+00
Benzo(a)pyrene	61.33643527	1.0484E-01	1.6433E+00
Benzo(b)fluoranthene	104.9909475	1.7946E-01	2.8129E+00
Benzo(g,h,i)perylene	6.655879888	1.1377E-02	1.7832E-01
Benzo(k)fluoranthene	10.87999323	1.8597E-02	2.9149E-01
Benzoic acid	5.006356559	8.5574E-03	1.3413E-01
bis(2-Chloroethoxy)methane	6.655879888	1.1377E-02	1.7832E-01
bis(2-Chloroethyl)ether	6.655879888	1.1377E-02	1.7832E-01
bis(2-Chloroisopropyl)ether	6.655879888	1.1377E-02	1.7832E-01
bis(2-Ethylhexyl)phthalate	86.07887249	1.4713E-01	2.3062E+00
Butane,1,1,3,4-Tetrachloro-	4.615064992	7.8885E-03	1.2364E-01
Butylbenzylphthalate	39.72844873	6.7908E-02	1.0644E+00
Carbazole	18.92344171	3.2346E-02	5.0699E-01
Carbon Disulfide	26.63560996	4.5528E-02	7.1361E-01
Chlorobenzene	3.844185056	6.5709E-03	1.0299E-01
Chloroethane	0.001764757	3.0165E-06	4.7280E-05
Chloromethane	0.206368875	3.5275E-04	5.5289E-03
Chrysene	155.1487311	2.6520E-01	4.1567E+00
Decane, 3,4-Dimethyl	0.094413059	1.6138E-04	2.5295E-03
Diacetone alcohol	2527.635596	4.3205E+00	6.7719E+01
Dibenz(a,h)anthracene	6.655879888	1.1377E-02	1.7832E-01
Dibenzofuran	189.6466875	3.2416E-01	5.0809E+00
Diethylphthalate	6.659079678	1.1382E-02	1.7841E-01
Dimethyl Disulfide	1.730906083	2.9586E-03	4.6374E-02
Dimethylphthalate	6.655879888	1.1377E-02	1.7832E-01
Di-n-butylphthalate	13.95355046	2.3851E-02	3.7384E-01
Di-n-octylphthalate	15.33901522	2.6219E-02	4.1096E-01
Eicosane	1.656689997	2.8318E-03	4.4385E-02
Ethyl cyanide	0.010999277	1.8801E-05	2.9469E-04
Ethylbenzene	45.67776881	7.8077E-02	1.2238E+00
Famphur	0.033997766	5.8112E-05	9.1085E-04
Fluoranthene	446.0559137	7.6244E-01	1.1951E+01
Fluorene	107.3916964	1.8356E-01	2.8772E+00
Heptadecane, 2,6,10,15-Tetra	2.011694997	3.4386E-03	5.3896E-02
Hexachlorobenzene	6.655879888	1.1377E-02	1.7832E-01
Hexachlorobutadiene	12.09928988	2.0681E-02	3.2416E-01
Hexachlorocyclopentadiene	6.655879888	1.1377E-02	1.7832E-01
Hexachloroethane	6.655879888	1.1377E-02	1.7832E-01
Indeno(1,2,3-cd)pyrene	6.655879888	1.1377E-02	1.7832E-01
Isobutyl alcohol	0.010999277	1.8801E-05	2.9469E-04
Isophorone	6.65827973	1.1381E-02	1.7839E-01
Isopropyl Alcohol/2-propanol	1.241278203	2.1217E-03	3.3256E-02
Kepone	58.03510406	9.9199E-02	1.5548E+00
Mesityl oxide	49.58236491	8.4751E-02	1.3284E+00

Table A-6. (continued).

Constituent	Total (kg)	5.8504E+08 (mg/kg)	0.0638 (mg/L)
Methyl Acetate	0.283239177	4.8414E-04	7.5884E-03
Methylene Chloride	48.91817499	8.3616E-02	1.3106E+00
Naphthalene	248.7161768	4.2513E-01	6.6635E+00
Nitrobenzene	6.655879888	1.1377E-02	1.7832E-01
N-Nitroso-di-n-propylamine	6.655879888	1.1377E-02	1.7832E-01
N-Nitrosodiphenylamine	6.655879888	1.1377E-02	1.7832E-01
Octane,2,3,7-Trimethyl	0.094413059	1.6138E-04	2.5295E-03
o-Toluenesulfonamide	2.958374995	5.0567E-03	7.9259E-02
Pentachlorophenol	32.69898432	5.5892E-02	8.7605E-01
Phenanthrene	683.4377181	1.1682E+00	1.8310E+01
Phenol	46.67445686	7.9781E-02	1.2505E+00
Phenol,2,6-Bis(1,1-Dimethyl)	2.366699996	4.0454E-03	6.3407E-02
p-Toluenesulfonamide	2.958374995	5.0567E-03	7.9259E-02
Pyrene	148.1681822	2.5326E-01	3.9696E+00
Styrene	0.000599961	1.0255E-06	1.6074E-05
Tetrachloroethene	5.637621485	9.6364E-03	1.5104E-01
Toluene	574.50195	9.8199E-01	1.5392E+01
Tributylphosphate	212.6773638	3.6353E-01	5.6979E+00
Trichloroethene	42.14465605	7.2038E-02	1.1291E+00
Undecane,4,6-Dimethyl-	0.094413059	1.6138E-04	2.5295E-03
Xylene (ortho)	2.271559432	3.8828E-03	6.0858E-02
Xylene (total)	2020.870091	3.4543E+00	5.4142E+01
		total mg/L=	2.9048E+02

* Assume H20 density = 1.064 (from PHREEQC) and mass moisture content = 6%)

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Appendix B

PHREEQC Input and Output Files

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B-1. PHREEQC Input File

```
TITLE Test Screened Constituents(assume 1L water, 16.7 kg soil), mix rain
and applied water, solubles as REACTION
SOLUTION 1 Average Rainfall Composition
        units   mg/L
        pH      5.6
        pe      8.451
        temp    25.0
        redox   O(0)/O(-2)
        O(0)            1.0     O2(g) -0.7
Na    2
K     0.27
Ca    0.13
Mg    0.27
C     0.36
Cl    3.8
S(6)  0.62
SOLUTION 2 INEEL Water Quality (CPP-1, 6/6/91)
units  mg/L
pH    8
pe    8.4
redox   O(0)/O(-2)
        O(0)            1.0     O2(g) -0.7
C     194
Ca    54
Mg    14
Na    7.9
K     2.5
Cl    18
S(6)  22
MIX 1 Mixing Solutions 1 and 2
1   0.85
2   0.15
SAVE SOLUTION  3
END
USE SOLUTION  3
REACTION
NaCN  2.16e-04
NaI   9.49e-07
1.0
EQUILIBRIUM_PHASES 1
Calcite    0.0  6.1
Illite     0.0   4.1
Kaolinite  0.0  0.0
Quartz     0.0  106.5
Gypsum     0.0   0.0013
Albite     0.0  14.4
K-Feldspar  0.0  7.8
Fluorapatite  0.0  0.017
```

```
Dolomite  0.0   Enstatite  21.7
Yb2O3  0.0  0.0094
Fe(OH)3  0.0  2.89
Pyrite  0.0  0.17
Zincite  0.0  Sphalerite  0.05
Birnessite  0.0  0.008
Barite  0.0  0.022
Borax  0.0  0.07
PuO2   0.0  8.76e-09
CaUO4  0.0  0.000417
Ca2V2O7  0.0  0.0035
Tb2O3    0.0  0.03
TcO2:2H2O(am)   0.0  5.72e-08
Ca3(AsO4)2  0.0  0.0006
Niter  0.0  0.001
Halite    0.0  0.0009
CaSeO4    0.0  1.8e-04
O2(g)   -0.7   1.0
CO2(g)    -3.5   1.0
END
```

B-2 PHREEQC Output File

```
Input file: C:\Documents\INEEL\pqe2\EDF274_update.pqi
  Output file: C:\Documents\INEEL\pqe2\EDF274_update.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive\llnl.dat

------------------
Reading data base.
------------------

      LLNL_AQUEOUS_MODEL_PARAMETERS
      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive\llnl.dat
      TITLE Test new Screening Assemblage (assume 1kg water, 6.2 kg soil),
mix rain and applied water, solubles as PHASES
      SOLUTION 1 Average Rainfall Composition
              units   mg/L
              pH      5.6
              pe      8.451
              temp    25.0
              redox   O(0)/O(-2)
              O(0)            1.0     O2(g) -0.7
      Na    2
      K     0.27
      Ca    0.13
      Mg    0.27
      C     0.36
      Cl    3.8
      S(6)  0.62
      SOLUTION 2 INEEL Water Quality (CPP-1, 6/6/91)
      units  mg/L
      pH    8
      pe     8.4
      redox   O(0)/O(-2)
              O(0)            1.0     O2(g) -0.7
      C     194
      Ca    54
      Mg    14
```

```
     Na    7.9
     K     2.5
     Cl    18
     S(6)  22
     MIX 1 Mixing Solutions 1 and 2
     1   0.85
     2   0.15
     SAVE SOLUTION  3
     END
-----
TITLE
-----

 Test new Screening Assemblage (assume 1kg water, 6.2 kg soil), mix rain
and applied water, solubles as PHASES

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.   Average Rainfall Composition

-----------------------Solution composition--------------------------------

     Elements           Molality       Moles

     C                5.902e-006  5.902e-006
     Ca               3.244e-006  3.244e-006
     Cl               1.072e-004  1.072e-004
     K                6.906e-006  6.906e-006
     Mg               1.111e-005  1.111e-005
     Na               8.700e-005  8.700e-005
     O(0)             5.113e-004  5.113e-004  Equilibrium with O2(g)
     S(6)             6.456e-006  6.456e-006

-----------------------Description of solution----------------------------

                                       pH  =   5.600
                                       pe  =   8.451
                          Activity of water  =   1.000
                             Ionic strength  =  1.438e-004
                           Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  = -1.669e-006
                        Total CO2 (mol/kg)  =  5.902e-006
                      Temperature (deg C)  =  25.000
                    Electrical balance (eq)  =  4.179e-006
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   1.70
                                Iterations  =   4
                                   Total H  = 1.110507e+002
```

Total O = 5.552587e+001

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	15.0007	0.8874

----------Distribution of species----------

Species	Molality	Log Activity	Molality	Log Activity	Log Gamma
H+	2.546e-006	2.512e-006	-5.594	-5.600	-0.006
OH-	3.889e-009	3.836e-009	-8.410	-8.416	-0.006
H2O	5.553e+001	1.000e+000	-0.000	-0.000	0.000
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-266.969	-266.969	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-239.283	-239.283	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-148.571	-148.571	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-51.542	-51.542	0.000
C(4)	5.902e-006				
CO2	5.027e-006	5.027e-006	-5.299	-5.299	0.000
HCO3-	8.748e-007	8.627e-007	-6.058	-6.064	-0.006
MgHCO3+	1.067e-010	1.052e-010	-9.972	-9.978	-0.006
NaHCO3	1.059e-010	1.059e-010	-9.975	-9.975	0.000
CaHCO3+	3.179e-011	3.136e-011	-10.498	-10.504	-0.006
CO3-2	1.611e-011	1.524e-011	-10.793	-10.817	-0.024
MgCO3	1.692e-013	1.692e-013	-12.771	-12.771	0.000

CaCO3	1.083e-013	1.083e-013	-12.965	-12.965	0.000
NaCO3-	4.638e-015	4.574e-015	-14.334	-14.340	-0.006
Ca	3.244e-006				
Ca+2	3.241e-006	3.067e-006	-5.489	-5.513	-0.024
CaSO4	2.725e-009	2.725e-009	-8.565	-8.565	0.000
CaCl+	6.967e-011	6.871e-011	-10.157	-10.163	-0.006
CaHCO3+	3.179e-011	3.136e-011	-10.498	-10.504	-0.006
CaOH+	1.749e-013	1.725e-013	-12.757	-12.763	-0.006
CaCO3	1.083e-013	1.083e-013	-12.965	-12.965	0.000
CaCl2	8.542e-015	8.542e-015	-14.068	-14.068	0.000
Cl(-1)	1.072e-004				
Cl-	1.072e-004	1.057e-004	-3.970	-3.976	-0.006
NaCl	1.594e-009	1.594e-009	-8.798	-8.798	0.000
MgCl+	8.786e-010	8.665e-010	-9.056	-9.062	-0.006
CaCl+	6.967e-011	6.871e-011	-10.157	-10.163	-0.006
HCl	5.963e-011	5.963e-011	-10.225	-10.225	0.000
KCl	2.417e-011	2.417e-011	-10.617	-10.617	0.000
CaCl2	8.542e-015	8.542e-015	-14.068	-14.068	0.000
Cl(1)	1.233e-019				
HClO	1.219e-019	1.219e-019	-18.914	-18.914	0.000
ClO-	1.327e-021	1.309e-021	-20.877	-20.883	-0.006
Cl(3)	2.103e-031				
ClO2-	2.095e-031	2.066e-031	-30.679	-30.685	-0.006
HClO2	7.674e-034	7.674e-034	-33.115	-33.115	0.000
Cl(5)	2.354e-027				
ClO3-	2.354e-027	2.321e-027	-26.628	-26.634	-0.006
Cl(7)	1.320e-027				
ClO4-	1.320e-027	1.301e-027	-26.880	-26.886	-0.006
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-44.302	-44.302	0.000
K	6.906e-006				
K+	6.905e-006	6.810e-006	-5.161	-5.167	-0.006
KSO4-	3.390e-010	3.343e-010	-9.470	-9.476	-0.006
KCl	2.417e-011	2.417e-011	-10.617	-10.617	0.000
KOH	9.400e-015	9.400e-015	-14.027	-14.027	0.000
KHSO4	7.410e-016	7.410e-016	-15.130	-15.130	0.000
Mg	1.111e-005				
Mg+2	1.109e-005	1.050e-005	-4.955	-4.979	-0.024
MgSO4	1.706e-008	1.706e-008	-7.768	-7.768	0.000
MgCl+	8.786e-010	8.665e-010	-9.056	-9.062	-0.006
MgHCO3+	1.067e-010	1.052e-010	-9.972	-9.978	-0.006
MgCO3	1.692e-013	1.692e-013	-12.771	-12.771	0.000
Mg4(OH)4+4	6.773e-038	5.429e-038	-37.169	-37.265	-0.096
Na	8.700e-005				
Na+	8.699e-005	8.579e-005	-4.061	-4.067	-0.006
NaSO4-	3.496e-009	3.448e-009	-8.456	-8.462	-0.006
NaCl	1.594e-009	1.594e-009	-8.798	-8.798	0.000
NaHCO3	1.059e-010	1.059e-010	-9.975	-9.975	0.000
NaOH	5.677e-014	5.677e-014	-13.246	-13.246	0.000
NaCO3-	4.638e-015	4.574e-015	-14.334	-14.340	-0.006
O(0)	5.113e-004				

O2	2.556e-004	2.556e-004	-3.592	-3.592	0.000
S(6)	6.456e-006				
SO4-2	6.430e-006	6.083e-006	-5.192	-5.216	-0.024
MgSO4	1.706e-008	1.706e-008	-7.768	-7.768	0.000
NaSO4-	3.496e-009	3.448e-009	-8.456	-8.462	-0.006
CaSO4	2.725e-009	2.725e-009	-8.565	-8.565	0.000
HSO4-	1.565e-009	1.543e-009	-8.805	-8.812	-0.006
KSO4-	3.390e-010	3.343e-010	-9.470	-9.476	-0.006
KHSO4	7.410e-016	7.410e-016	-15.130	-15.130	0.000
H2SO4	3.658e-018	3.658e-018	-17.437	-17.437	0.000

----------Saturation indices----------

Phase	SI	log IAP	log KT	
Anhydrite	-6.38	-10.73	-4.35	CaSO4
Antarcticite	-17.56	-13.47	4.09	CaCl2:6H2O
Aphthitalite	-26.11	-30.00	-3.89	NaK3(SO4)2
Aragonite	-7.95	-5.98	1.97	CaCO3
Arcanite	-13.71	-15.55	-1.84	K2SO4
Artinite	-18.85	0.78	19.63	Mg2CO3(OH)2:3H2O
Bassanite	-7.02	-10.73	-3.71	CaSO4:0.5H2O
Bischofite	-17.32	-12.93	4.39	MgCl2:6H2O
Bloedite	-21.07	-23.54	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-10.06	6.22	16.28	Mg(OH)2
Burkeite	-44.78	-35.30	9.49	Na6CO3(SO4)2
C	-72.22	-8.07	64.15	C
C(g)	-189.84	-8.07	181.77	C
Ca	-132.35	7.48	139.83	Ca
Ca(g)	-157.59	7.48	165.07	Ca
Ca2Cl2(OH)2:H2O	-34.07	-7.78	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-64.73	3.59	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-7.80	-5.98	1.82	CaCO3
Carnallite	-26.35	-22.07	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-7.19	-10.73	-3.54	CaSO4:0.5H2O
CH4(g)	-145.73	-4.48	141.25	CH4
Chloromagnesite	-34.75	-12.93	21.82	MgCl2
Cl2(g)	-23.94	-20.95	2.99	Cl2
CO(g)	-48.54	-9.87	38.68	CO
CO2(g)	-3.84	-11.66	-7.83	CO2
Dolomite	-13.89	-11.42	2.47	CaMg(CO3)2
Dolomite-dis	-15.43	-11.42	4.01	CaMg(CO3)2
Dolomite-ord	-13.88	-11.42	2.46	CaMg(CO3)2
Epsomite	-8.23	-10.19	-1.96	MgSO4:7H2O
Gaylussite	-25.74	-14.57	11.16	CaNa2(CO3)2:5H2O
Glauberite	-18.61	-24.08	-5.47	Na2Ca(SO4)2
Gypsum	-6.20	-10.73	-4.53	CaSO4:2H2O
H2(g)	-41.20	1.80	43.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-9.61	-8.04	1.56	NaCl
HCl(g)	-15.88	-9.58	6.30	HCl
Hexahydrite	-8.47	-10.19	-1.73	MgSO4:6H2O

Huntite	-32.52	-22.31	10.22	CaMg3(CO3)4
Hydromagnesite	-46.29	-15.55	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-25.21	-13.47	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-69.65	1.33	70.98	K
K(g)	-80.25	1.33	81.58	K
K2CO3:1.5H2O	-24.18	-10.80	13.38	K2CO3:1.5H2O
K2O	-83.17	0.87	84.04	K2O
K3H(SO4)2	-27.91	-31.53	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-94.23	-66.52	27.71	K8H4(CO3)6:3H2O
Kainite	-19.03	-19.34	-0.31	KMgClSO4:3H2O
Kalicinite	-11.51	-11.23	0.28	KHCO3
Kieserite	-9.93	-10.19	-0.27	MgSO4:H2O
KMgCl3	-43.32	-22.07	21.25	KMgCl3
KMgCl3:2H2O	-36.04	-22.07	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-19.96	-9.70	10.26	KNaCO3:6H2O
Lansfordite	-10.28	-5.44	4.84	MgCO3:5H2O
Leonite	-21.63	-25.74	-4.11	K2Mg(SO4)2:4H2O
Lime	-26.88	5.69	32.57	CaO
Magnesite	-7.72	-5.44	2.27	MgCO3
Mercallite	-14.54	-15.98	-1.44	KHSO4
Mg	-114.50	8.02	122.52	Mg
Mg(g)	-134.23	8.02	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-13.83	-8.64	5.20	
Mg1.25SO4(OH)0.5:0.5H2O				
Mg1.5SO4(OH)	-16.29	-7.08	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-25.66	-12.93	12.73	MgCl2:2H2O
MgCl2:4H2O	-20.23	-12.93	7.30	MgCl2:4H2O
MgCl2:H2O	-29.00	-12.93	16.07	MgCl2:H2O
MgOHCl	-19.25	-3.35	15.89	MgOHCl
MgSO4	-15.02	-10.19	4.83	MgSO4
Mirabilite	-12.19	-13.35	-1.15	Na2SO4:10H2O
Misenite	-100.37	-111.45	-11.08	K8H6(SO4)7
Monohydrocalcite	-8.66	-5.98	2.68	CaCO3:H2O
Na	-64.94	2.43	67.37	Na
Na(g)	-78.43	2.43	80.86	Na
Na2CO3	-19.76	-8.60	11.16	Na2CO3
Na2CO3:7H2O	-18.54	-8.60	9.94	Na2CO3:7H2O
Na2O	-64.35	3.07	67.42	Na2O
Na3H(SO4)2	-27.34	-28.23	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-31.53	-37.43	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-9.99	-10.13	-0.14	NaHCO3
Natron	-18.19	-8.60	9.59	Na2CO3:10H2O
Nesquehonite	-10.73	-5.44	5.29	MgCO3:3H2O
O2(g)	-0.70	-3.59	-2.89	O2
Oxychloride-Mg	-22.97	2.87	25.83	Mg2Cl(OH)3:4H2O
Pentahydrite	-8.81	-10.19	-1.39	MgSO4:5H2O
Periclase	-15.10	6.22	21.33	MgO
Picromerite	-21.30	-25.74	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-25.90	-14.57	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-32.89	-47.20	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-16.86	5.69	22.55	Ca(OH)2
Starkeyite	-9.19	-10.19	-1.00	MgSO4:4H2O

```
      Sylvite          -9.97   -9.14    0.83  KCl
      Syngenite       -18.68  -26.28   -7.60  K2Ca(SO4)2:H2O
      Tachyhydrite    -56.47  -39.33   17.14  Mg2CaCl6:12H2O
      Thenardite      -12.99  -13.35   -0.36  Na2SO4
      Thermonatrite   -19.53   -8.60   10.94  Na2CO3:H2O
      Trona-K         -32.52  -20.93   11.59  K2NaH(CO3)2:2H2O

Initial solution 2.   INEEL Water Quality (CPP-1, 6/6/91)

-----------------Solution composition------------------------------

      Elements           Molality       Moles

      C                3.181e-003  3.181e-003
      Ca               1.348e-003  1.348e-003
      Cl               5.079e-004  5.079e-004
      K                6.396e-005  6.396e-005
      Mg               5.762e-004  5.762e-004
      Na               3.437e-004  3.437e-004
      O(0)             5.105e-004  5.105e-004  Equilibrium with
O2(g)
      S(6)             2.291e-004  2.291e-004

-----------------Description of solution---------------------------

                                       pH  =   8.000
                                       pe  =   8.400
                          Activity of water  =   1.000
                             Ionic strength  =  6.037e-003
                          Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  3.167e-003
                       Total CO2 (mol/kg)  =  3.181e-003
                     Temperature (deg C)  =  25.000
                   Electrical balance (eq)  =  1.228e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   1.53
                                 Iterations  =   5
                                    Total H  = 1.110537e+002
                                    Total O  = 5.553623e+001

----------------------Redox couples--------------------------------

      Redox couple             pe  Eh (volts)

      O(-2)/O(0)          12.6007      0.7454
```

----------Distribution of species----------

Species	Molality	Log Activity	Molality	Log Activity	Log Gamma
OH-	1.047e-006	9.634e-007	-5.980	-6.016	-0.036
H+	1.077e-008	1.000e-008	-7.968	-8.000	-0.032
H2O	5.553e+001	9.999e-001	-0.000	-0.000	0.000
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-264.752	-264.752	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-237.066	-237.066	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-147.463	-147.463	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-50.433	-50.433	0.000
C(4)	3.181e-003				
HCO3-	3.020e-003	2.781e-003	-2.520	-2.556	-0.036
CO2	6.441e-005	6.451e-005	-4.191	-4.190	0.001
CaHCO3+	3.309e-005	3.047e-005	-4.480	-4.516	-0.036
CaCO3	2.644e-005	2.644e-005	-4.578	-4.578	0.000
CO3-2	1.712e-005	1.234e-005	-4.766	-4.909	-0.142
MgHCO3+	1.403e-005	1.292e-005	-4.853	-4.889	-0.036
MgCO3	5.221e-006	5.221e-006	-5.282	-5.282	0.000
NaHCO3	1.253e-006	1.253e-006	-5.902	-5.902	0.000
NaCO3-	1.477e-008	1.360e-008	-7.831	-7.866	-0.036
Ca	1.348e-003				
Ca+2	1.269e-003	9.247e-004	-2.896	-3.034	-0.138
CaHCO3+	3.309e-005	3.047e-005	-4.480	-4.516	-0.036
CaCO3	2.644e-005	2.644e-005	-4.578	-4.578	0.000
CaSO4	1.890e-005	1.890e-005	-4.724	-4.724	0.000
CaCl+	9.928e-008	9.143e-008	-7.003	-7.039	-0.036
CaOH+	1.418e-008	1.306e-008	-7.848	-7.884	-0.036
CaCl2	5.017e-011	5.017e-011	-10.300	-10.300	0.000
Cl(-1)	5.079e-004				
Cl-	5.076e-004	4.665e-004	-3.294	-3.331	-0.037
MgCl+	1.582e-007	1.457e-007	-6.801	-6.837	-0.036
CaCl+	9.928e-008	9.143e-008	-7.003	-7.039	-0.036
NaCl	2.583e-008	2.583e-008	-7.588	-7.588	0.000
KCl	9.198e-010	9.198e-010	-9.036	-9.036	0.000
CaCl2	5.017e-011	5.017e-011	-10.300	-10.300	0.000
HCl	1.048e-012	1.048e-012	-11.980	-11.980	0.000
Cl(1)	8.416e-021				
ClO-	6.274e-021	5.777e-021	-20.202	-20.238	-0.036
HClO	2.143e-021	2.143e-021	-20.669	-20.669	0.000
Cl(3)	9.904e-031				
ClO2-	9.904e-031	9.120e-031	-30.004	-30.040	-0.036
HClO2	1.348e-035	1.348e-035	-34.870	-34.870	0.000
Cl(5)	1.114e-026				
ClO3-	1.114e-026	1.024e-026	-25.953	-25.990	-0.036
Cl(7)	6.244e-027				
ClO4-	6.244e-027	5.744e-027	-26.205	-26.241	-0.036

H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-44.302	-44.302	0.001
K	6.396e-005				
K+	6.389e-005	5.872e-005	-4.195	-4.231	-0.037
KSO4-	7.201e-008	6.631e-008	-7.143	-7.178	-0.036
KCl	9.198e-010	9.198e-010	-9.036	-9.036	0.000
KOH	2.036e-011	2.036e-011	-10.691	-10.691	0.000
KHSO4	5.851e-016	5.851e-016	-15.233	-15.233	0.000
Mg	5.762e-004				
Mg+2	5.418e-004	4.001e-004	-3.266	-3.398	-0.132
MgSO4	1.495e-005	1.495e-005	-4.825	-4.825	0.000
MgHCO3+	1.403e-005	1.292e-005	-4.853	-4.889	-0.036
MgCO3	5.221e-006	5.221e-006	-5.282	-5.282	0.000
MgCl+	1.582e-007	1.457e-007	-6.801	-6.837	-0.036
Mg4(OH)4+4	1.643e-021	4.554e-022	-20.784	-21.342	-0.557
Na	3.437e-004				
Na+	3.421e-004	3.151e-004	-3.466	-3.502	-0.036
NaHCO3	1.253e-006	1.253e-006	-5.902	-5.902	0.000
NaSO4-	3.163e-007	2.912e-007	-6.500	-6.536	-0.036
NaCl	2.583e-008	2.583e-008	-7.588	-7.588	0.000
NaCO3-	1.477e-008	1.360e-008	-7.831	-7.866	-0.036
NaOH	5.236e-011	5.236e-011	-10.281	-10.281	0.000
O(0)	5.105e-004				
O2	2.553e-004	2.556e-004	-3.593	-3.592	0.001
S(6)	2.291e-004				
SO4-2	1.949e-004	1.399e-004	-3.710	-3.854	-0.144
CaSO4	1.890e-005	1.890e-005	-4.724	-4.724	0.000
MgSO4	1.495e-005	1.495e-005	-4.825	-4.825	0.000
NaSO4-	3.163e-007	2.912e-007	-6.500	-6.536	-0.036
KSO4-	7.201e-008	6.631e-008	-7.143	-7.178	-0.036
HSO4-	1.535e-010	1.413e-010	-9.814	-9.850	-0.036
KHSO4	5.851e-016	5.851e-016	-15.233	-15.233	0.000
H2SO4	1.333e-021	1.333e-021	-20.875	-20.875	0.000

--------------------Saturation indices--------------------------------

Phase	SI	log IAP	log KT	
Anhydrite	-2.54	-6.89	-4.35	CaSO4
Antarcticite	-13.79	-9.70	4.09	CaCl2:6H2O
Aphthitalite	-20.02	-23.90	-3.89	NaK3(SO4)2
Aragonite	0.44	2.41	1.97	CaCO3
Arcanite	-10.47	-12.32	-1.84	K2SO4
Artinite	-4.98	14.65	19.63	Mg2CO3(OH)2:3H2O
Bassanite	-3.18	-6.89	-3.71	CaSO4:0.5H2O
Bischofite	-14.45	-10.06	4.39	MgCl2:6H2O
Bloedite	-15.63	-18.11	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-3.68	12.60	16.28	Mg(OH)2
Burkeite	-32.76	-23.27	9.49	Na6CO3(SO4)2
C	-71.11	-6.96	64.15	C
C(g)	-188.73	-6.96	181.77	C
Ca	-125.07	14.76	139.83	Ca

```
      Ca(g)           -150.31   14.76  165.07  Ca
      Ca2Cl2(OH)2:H2O -23.02    3.27   26.29  Ca2Cl2(OH)2:H2O
      Ca4Cl2(OH)6:13H2O -39.13   29.20   68.33  Ca4Cl2(OH)6:13H2O
      Calcite           0.59    2.41    1.82  CaCO3
      Carnallite      -21.89  -17.62    4.27  KMgCl3:6H2O
      CaSO4:0.5H2O(beta)  -3.35   -6.89   -3.54  CaSO4:0.5H2O
      CH4(g)          -144.62   -3.37  141.25  CH4
      Chloromagnesite -31.88  -10.06   21.82  MgCl2
      Cl2(g)          -27.45  -24.46    2.99  Cl2
      CO(g)           -47.44   -8.76   38.68  CO
      CO2(g)           -2.73  -10.56   -7.83  CO2
      Dolomite          1.98    4.46    2.47  CaMg(CO3)2
      Dolomite-dis      0.44    4.46    4.01  CaMg(CO3)2
      Dolomite-ord      1.99    4.46    2.46  CaMg(CO3)2
      Epsomite         -5.29   -7.25   -1.96  MgSO4:7H2O
      Gaylussite      -10.31    0.85   11.16  CaNa2(CO3)2:5H2O
      Glauberite      -12.28  -17.75   -5.47  Na2Ca(SO4)2
      Gypsum           -2.36   -6.89   -4.53  CaSO4:2H2O
      H2(g)           -41.20    1.80   43.00  H2
      H2O(g)           -1.59   -0.00    1.59  H2O
      Halite           -8.40   -6.83    1.56  NaCl
      HCl(g)          -17.63  -11.33    6.30  HCl
      Hexahydrite      -5.53   -7.25   -1.73  MgSO4:6H2O
      Huntite          -1.67    8.55   10.22  CaMg3(CO3)4
      Hydromagnesite   -9.95   20.79   30.74  Mg5(CO3)4(OH)2:4H2O
      Hydrophilite    -21.44   -9.70   11.75  CaCl2
      Ice              -0.14   -0.00    0.14  H2O
      K               -66.31    4.67   70.98  K
      K(g)            -76.91    4.67   81.58  K
      K2CO3:1.5H2O    -16.40   -3.02   13.38  K2CO3:1.5H2O
      K2O             -76.50    7.54   84.04  K2O
      K3H(SO4)2       -24.78  -28.40   -3.62  K3H(SO4)2
      K8H4(CO3)6:3H2O -60.89  -33.19   27.71  K8H4(CO3)6:3H2O
      Kainite         -14.50  -14.81   -0.31  KMgClSO4:3H2O
      Kalicinite       -7.07   -6.79    0.28  KHCO3
      Kieserite        -6.99   -7.25   -0.27  MgSO4:H2O
      KMgCl3          -38.87  -17.62   21.25  KMgCl3
      KMgCl3:2H2O     -31.58  -17.62   13.96  KMgCl3:2H2O
      KNaCO3:6H2O     -12.55   -2.29   10.26  KNaCO3:6H2O

      Lansfordite      -2.79    2.05    4.84  MgCO3:5H2O
      Leonite         -15.46  -19.57   -4.11  K2Mg(SO4)2:4H2O
      Lime            -19.60   12.97   32.57  CaO
      Magnesite        -0.23    2.05    2.27  MgCO3
      Mercallite      -14.65  -16.09   -1.44  KHSO4
      Mg             -108.12   14.40  122.52  Mg
      Mg(g)          -127.85   14.40  142.25  Mg
      Mg1.25SO4(OH)0.5:0.5H2O  -9.30   -4.10    5.20
Mg1.25SO4(OH)0.5:0.5H2O
      Mg1.5SO4(OH)    -10.16   -0.95    9.21  Mg1.5SO4(OH)
      MgCl2:2H2O      -22.79  -10.06   12.73  MgCl2:2H2O
      MgCl2:4H2O      -17.36  -10.06    7.30  MgCl2:4H2O
```

MgCl2:H2O	-26.13	-10.06	16.07	MgCl2:H2O
MgOHCl	-14.62	1.27	15.89	MgOHCl
MgSO4	-12.08	-7.25	4.83	MgSO4
Mirabilite	-9.70	-10.86	-1.15	Na2SO4:10H2O
Misenite	-97.75	-108.83	-11.08	K8H6(SO4)7
Monohydrocalcite	-0.27	2.41	2.68	CaCO3:H2O
Na	-61.97	5.40	67.37	Na
Na(g)	-75.46	5.40	80.86	Na
Na2CO3	-12.72	-1.56	11.16	Na2CO3
Na2CO3:7H2O	-11.50	-1.56	9.94	Na2CO3:7H2O
Na2O	-58.42	9.00	67.42	Na2O
Na3H(SO4)2	-25.32	-26.21	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-22.71	-28.60	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-5.92	-6.06	-0.14	NaHCO3
Natron	-11.15	-1.56	9.59	Na2CO3:10H2O
Nesquehonite	-3.24	2.05	5.29	MgCO3:3H2O
O2(g)	-0.70	-3.59	-2.89	O2
Oxychloride-Mg	-11.96	13.87	25.83	Mg2Cl(OH)3:4H2O
Pentahydrite	-5.87	-7.25	-1.39	MgSO4:5H2O
Periclase	-8.72	12.60	21.33	MgO
Picromerite	-15.13	-19.57	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-10.47	0.85	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-19.03	-33.35	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-9.58	12.97	22.55	Ca(OH)2
Starkeyite	-6.25	-7.25	-1.00	MgSO4:4H2O
Sylvite	-8.39	-7.56	0.83	KCl
Syngenite	-11.60	-19.20	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-46.96	-29.82	17.14	Mg2CaCl6:12H2O
Thenardite	-10.50	-10.86	-0.36	Na2SO4
Thermonatrite	-12.50	-1.56	10.94	Na2CO3:H2O
Trona-K	-20.66	-9.08	11.59	K2NaH(CO3)2:2H2O

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-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using mix 1.    Mixing Solutions 1 and 2
Mixture 1. Mixing Solutions 1 and 2

 8.500e-001 Solution 1     Average Rainfall Composition
 1.500e-001 Solution 2     INEEL Water Quality (CPP-1, 6/6/91)

-----------------Solution composition------------------------------
```

Elements	Molality	Moles
C	4.822e-004	4.822e-004
Ca	2.049e-004	2.049e-004
Cl	1.673e-004	1.673e-004

K	1.546e-005	1.546e-005
Mg	9.587e-005	9.587e-005
Na	1.255e-004	1.255e-004
S	3.986e-005	3.986e-005

----------Description of solution----------

pH = 7.929 Charge balance
pe = 12.671 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 1.062e-003
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = 4.736e-004
Total CO2 (mol/kg) = 4.822e-004
Temperature (deg C) = 25.000
Electrical balance (eq) = 2.197e-005
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.51
Iterations = 14
Total H = 1.110511e+002
Total O = 5.552743e+001

----------Distribution of species----------

Species	Molality	Log Activity	Molality	Log Activity	Log Gamma
OH-	8.493e-007	8.185e-007	-6.071	-6.087	-0.016
H+	1.219e-008	1.177e-008	-7.914	-7.929	-0.015
H2O	5.553e+001	1.000e+000	-0.000	-0.000	0.000
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-266.194	-266.194	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-238.509	-238.509	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-148.184	-148.184	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-51.155	-51.155	0.000
C(4)	4.822e-004				
HCO3-	4.657e-004	4.489e-004	-3.332	-3.348	-0.016
CO2	1.225e-005	1.226e-005	-4.912	-4.912	0.000
CO3-2	1.959e-006	1.692e-006	-5.708	-5.772	-0.064
CaHCO3+	9.671e-007	9.322e-007	-6.015	-6.030	-0.016
CaCO3	6.872e-007	6.872e-007	-6.163	-6.163	0.000
MgHCO3+	4.440e-007	4.280e-007	-6.353	-6.369	-0.016
MgCO3	1.469e-007	1.469e-007	-6.833	-6.833	0.000
NaHCO3	7.761e-008	7.761e-008	-7.110	-7.110	0.000
NaCO3-	7.423e-010	7.156e-010	-9.129	-9.145	-0.016
Ca	2.049e-004				
Ca+2	2.024e-004	1.752e-004	-3.694	-3.756	-0.063
CaHCO3+	9.671e-007	9.322e-007	-6.015	-6.030	-0.016
CaSO4	8.454e-007	8.454e-007	-6.073	-6.073	0.000
CaCO3	6.872e-007	6.872e-007	-6.163	-6.163	0.000

CaCl+	6.211e-009	5.987e-009	-8.207	-8.223	-0.016
CaOH+	2.182e-009	2.103e-009	-8.661	-8.677	-0.016
CaCl2	1.135e-012	1.135e-012	-11.945	-11.945	0.000
Cl(-1)	1.673e-004				
Cl-	1.673e-004	1.612e-004	-3.777	-3.793	-0.016
MgCl+	1.072e-008	1.033e-008	-7.970	-7.986	-0.016
CaCl+	6.211e-009	5.987e-009	-8.207	-8.223	-0.016
NaCl	3.424e-009	3.424e-009	-8.465	-8.465	0.000
KCl	8.063e-011	8.063e-011	-10.093	-10.093	0.000
CaCl2	1.135e-012	1.135e-012	-11.945	-11.945	0.000
HCl	4.261e-013	4.261e-013	-12.370	-12.370	0.000
Cl(1)	2.942e-021				
ClO-	2.071e-021	1.996e-021	-20.684	-20.700	-0.016
HClO	8.713e-022	8.713e-022	-21.060	-21.060	0.000
Cl(3)	3.269e-031				
ClO2-	3.269e-031	3.151e-031	-30.486	-30.502	-0.016
HClO2	5.483e-036	5.483e-036	-35.261	-35.261	0.000
Cl(5)	3.673e-027				
ClO3-	3.673e-027	3.540e-027	-26.435	-26.451	-0.016
Cl(7)	2.059e-027				
ClO4-	2.059e-027	1.985e-027	-26.686	-26.702	-0.016
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-44.302	-44.302	0.000
K	1.546e-005				
K+	1.546e-005	1.490e-005	-4.811	-4.827	-0.016
KSO4-	4.119e-009	3.971e-009	-8.385	-8.401	-0.016
KCl	8.063e-011	8.063e-011	-10.093	-10.093	0.000
KOH	4.388e-012	4.388e-012	-11.358	-11.358	0.000
KHSO4	4.124e-017	4.124e-017	-16.385	-16.385	0.000
Mg	9.587e-005				
Mg+2	9.455e-005	8.209e-005	-4.024	-4.086	-0.061
MgSO4	7.239e-007	7.239e-007	-6.140	-6.140	0.000
MgHCO3+	4.440e-007	4.280e-007	-6.353	-6.369	-0.016
MgCO3	1.469e-007	1.469e-007	-6.833	-6.833	0.000
MgCl+	1.072e-008	1.033e-008	-7.970	-7.986	-0.016
Mg4(OH)4+4	7.510e-025	4.206e-025	-24.124	-24.376	-0.252
Na	1.255e-004				
Na+	1.254e-004	1.209e-004	-3.902	-3.918	-0.016
NaHCO3	7.761e-008	7.761e-008	-7.110	-7.110	0.000
NaSO4-	2.736e-008	2.637e-008	-7.563	-7.579	-0.016
NaCl	3.424e-009	3.424e-009	-8.465	-8.465	0.000
NaCO3-	7.423e-010	7.156e-010	-9.129	-9.145	-0.016
NaOH	1.707e-011	1.707e-011	-10.768	-10.768	0.000
O(0)	5.112e-004				
O2	2.556e-004	2.556e-004	-3.592	-3.592	0.000
S3O6-2	0.000e+000	0.000e+000	-183.903	-183.967	-0.064
S2-2	0.000e+000	0.000e+000	-255.491	-255.555	-0.064
S4O6-2	0.000e+000	0.000e+000	-277.572	-277.636	-0.064
S3-2	0.000e+000	0.000e+000	-362.583	-362.646	-0.064
S5O6-2	0.000e+000	0.000e+000	-400.120	-400.184	-0.064
S4-2	0.000e+000	0.000e+000	-469.901	-469.965	-0.064

S5-2	0.000e+000	0.000e+000	-577.436	-577.500	-0.064
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-143.492	-143.508	-0.016
H2S	0.000e+000	0.000e+000	-144.428	-144.428	0.000
S-2	0.000e+000	0.000e+000	-148.442	-148.505	-0.063
S2-2	0.000e+000	0.000e+000	-255.491	-255.555	-0.064
S3-2	0.000e+000	0.000e+000	-362.583	-362.646	-0.064
S4-2	0.000e+000	0.000e+000	-469.901	-469.965	-0.064
S5-2	0.000e+000	0.000e+000	-577.436	-577.500	-0.064
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-151.046	-151.110	-0.064
HS2O3-	0.000e+000	0.000e+000	-158.009	-158.025	-0.016
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-140.267	-140.331	-0.063
S(4)	0.000e+000				
SO3-2	0.000e+000	0.000e+000	-49.239	-49.303	-0.064
HSO3-	0.000e+000	0.000e+000	-49.985	-50.000	-0.016
H2SO3	0.000e+000	0.000e+000	-55.948	-55.948	0.000
SO2	0.000e+000	0.000e+000	-56.048	-56.048	0.000
S2O5-2	0.000e+000	0.000e+000	-104.767	-104.831	-0.064
S3O6-2	0.000e+000	0.000e+000	-183.903	-183.967	-0.064
S4O6-2	0.000e+000	0.000e+000	-277.572	-277.636	-0.064
S5O6-2	0.000e+000	0.000e+000	-400.120	-400.184	-0.064
S(5)	0.000e+000				
S2O6-2	0.000e+000	0.000e+000	-74.329	-74.393	-0.064
S(6)	3.986e-005				
SO4-2	3.826e-005	3.302e-005	-4.417	-4.481	-0.064
CaSO4	8.454e-007	8.454e-007	-6.073	-6.073	0.000
MgSO4	7.239e-007	7.239e-007	-6.140	-6.140	0.000
NaSO4-	2.736e-008	2.637e-008	-7.563	-7.579	-0.016
KSO4-	4.119e-009	3.971e-009	-8.385	-8.401	-0.016
HSO4-	4.073e-011	3.926e-011	-10.390	-10.406	-0.016
KHSO4	4.124e-017	4.124e-017	-16.385	-16.385	0.000
H2SO4	4.360e-022	4.360e-022	-21.360	-21.360	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-49.008	-49.072	-0.064
S(8)	3.538e-032				
HSO5-	3.538e-032	3.410e-032	-31.451	-31.467	-0.016

----------Saturation indices----------

Phase	SI	log IAP	log KT	
Anhydrite	-3.89	-8.24	-4.35	CaSO4
Antarcticite	-15.44	-11.34	4.09	CaCl2:6H2O
Aphthitalite	-23.47	-27.36	-3.89	NaK3(SO4)2
Aragonite	-1.15	0.82	1.97	CaCO3
Arcanite	-12.29	-14.13	-1.84	K2SO4
Artinite	-7.36	12.27	19.63	Mg2CO3(OH)2:3H2O
Bassanite	-4.53	-8.24	-3.71	CaSO4:0.5H2O
Bischofite	-16.06	-11.67	4.39	MgCl2:6H2O
Bloedite	-18.41	-20.88	-2.48	Na2Mg(SO4)2:4H2O

Brucite	-4.51	11.77	16.28	Mg(OH)2
Burkeite	-37.37	-27.89	9.49	Na6CO3(SO4)2
C	-71.83	-93.68	-21.85	C
C(g)	-189.45	-93.68	95.77	C
Ca	-125.93	-29.10	96.83	Ca
Ca(g)	-151.17	-29.10	122.07	Ca
Ca2Cl2(OH)2:H2O	-25.53	0.76	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-43.36	24.96	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-1.00	0.82	1.82	CaCO3
Carnallite	-24.56	-20.29	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-4.70	-8.24	-3.54	CaSO4:0.5H2O
CH4(g)	-145.34	-176.08	-30.74	CH4
Chloromagnesite	-33.49	-11.67	21.82	MgCl2
Cl2(g)	-28.23	17.76	45.99	Cl2
CO(g)	-48.16	-52.48	-4.32	CO
CO2(g)	-3.45	-11.28	-7.83	CO2
Dolomite	-1.15	1.32	2.47	CaMg(CO3)2
Dolomite-dis	-2.69	1.32	4.01	CaMg(CO3)2
Dolomite-ord	-1.14	1.32	2.46	CaMg(CO3)2
Epsomite	-6.60	-8.57	-1.96	MgSO4:7H2O
Gaylussite	-13.59	-2.43	11.16	CaNa2(CO3)2:5H2O
Glauberite	-15.09	-20.55	-5.47	Na2Ca(SO4)2
Gypsum	-3.71	-8.24	-4.53	CaSO4:2H2O
H2(g)	-41.20	-41.20	-0.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-143.45	-185.15	-41.70	H2S
Halite	-9.27	-7.71	1.56	NaCl
HCl(g)	-18.02	-11.72	6.30	HCl
Hexahydrite	-6.84	-8.57	-1.73	MgSO4:6H2O
Huntite	-7.91	2.31	10.22	CaMg3(CO3)4
Hydromagnesite	-16.98	13.76	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-23.09	-11.34	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-66.98	-17.50	49.48	K
K(g)	-77.58	-17.50	60.08	K
K2CO3:1.5H2O	-18.45	-5.07	13.38	K2CO3:1.5H2O
K2O	-77.83	6.20	84.04	K2O
K3H(SO4)2	-27.75	-31.37	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-70.55	-42.84	27.71	K8H4(CO3)6:3H2O
Kainite	-16.88	-17.19	-0.31	KMgClSO4:3H2O
Kalicinite	-8.46	-8.17	0.28	KHCO3
Kieserite	-8.30	-8.57	-0.27	MgSO4:H2O
KMgCl3	-41.54	-20.29	21.25	KMgCl3
KMgCl3:2H2O	-34.25	-20.29	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-14.42	-4.16	10.26	KNaCO3:6H2O
Lansfordite	-4.35	0.50	4.84	MgCO3:5H2O
Leonite	-18.59	-22.70	-4.11	K2Mg(SO4)2:4H2O
Lime	-20.47	12.10	32.57	CaO
Magnesite	-1.78	0.50	2.27	MgCO3
Mercallite	-15.80	-17.24	-1.44	KHSO4
Mg	-108.95	-29.43	79.52	Mg
Mg(g)	-128.68	-29.43	99.25	Mg

```
      Mg1.25SO4(OH)0.5:0.5H2O -10.82   -5.62    5.20
Mg1.25SO4(OH)0.5:0.5H2O
      Mg1.5SO4(OH)    -11.89   -2.68    9.21  Mg1.5SO4(OH)
      MgCl2:2H2O      -24.40  -11.67   12.73  MgCl2:2H2O
      MgCl2:4H2O      -18.97  -11.67    7.30  MgCl2:4H2O
      MgCl2:H2O       -27.74  -11.67   16.07  MgCl2:H2O
      MgOHCl          -15.84    0.05   15.89  MgOHCl
      MgSO4           -13.40   -8.57    4.83  MgSO4
      Mirabilite      -11.16  -12.32   -1.15  Na2SO4:10H2O
      Misenite       -106.48 -117.56  -11.08  K8H6(SO4)7
      Monohydrocalcite  -1.85    0.82    2.68  CaCO3:H2O
      Na              -62.46  -16.59   45.87  Na
      Na(g)           -75.95  -16.59   59.36  Na
      Na2CO3          -14.42   -3.25   11.16  Na2CO3
      Na2CO3:7H2O     -13.19   -3.25    9.94  Na2CO3:7H2O
      Na2O            -59.39    8.02   67.42  Na2O
      Na3H(SO4)2      -27.75  -28.64   -0.89  Na3H(SO4)2
      Na4Ca(SO4)3:2H2O -26.98  -32.87   -5.89  Na4Ca(SO4)3:2H2O
      Nahcolite        -7.12   -7.27   -0.14  NaHCO3
      Natron          -12.84   -3.25    9.59  Na2CO3:10H2O
      Nesquehonite     -4.79    0.50    5.29  MgCO3:3H2O
      O2(g)            -0.70   82.40   83.10  O2
      Oxychloride-Mg  -14.01   11.82   25.83  Mg2Cl(OH)3:4H2O
      Pentahydrite     -7.18   -8.57   -1.39  MgSO4:5H2O
      Periclase        -9.55   11.77   21.33  MgO
      Picromerite     -18.26  -22.70   -4.44  K2Mg(SO4)2:6H2O
      Pirssonite      -13.75   -2.43   11.32  Na2Ca(CO3)2:2H2O
      Polyhalite      -24.86  -39.18  -14.31  K2MgCa2(SO4)4:2H2O
      Portlandite     -10.44   12.10   22.55  Ca(OH)2
      S              -108.12 -143.94  -35.82  S
      S2(g)          -230.14 -287.89  -57.75  S2
      SO2(g)          -56.22  -61.54   -5.32  SO2
      Starkeyite       -7.57   -8.57   -1.00  MgSO4:4H2O
      Sylvite          -9.45   -8.62    0.83  KCl
      Syngenite       -14.77  -22.37   -7.60  K2Ca(SO4)2:H2O
      Tachyhydrite    -51.83  -34.68   17.14  Mg2CaCl6:12H2O
      Thenardite      -11.96  -12.32   -0.36  Na2SO4
      Thermonatrite   -14.19   -3.25   10.94  Na2CO3:H2O
      Trona-K         -23.93  -12.34   11.59  K2NaH(CO3)2:2H2O

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

      USE SOLUTION  3
      REACTION
      NaCN  2.16e-04
      NaI   9.49e-07
      1.0
```

```
      EQUILIBRIUM_PHASES 1
      Calcite    0.0  6.1
      Illite     0.0   4.1
      Kaolinite  0.0  0.0
      Quartz     0.0  106.5
      Gypsum     0.0   0.0013
      Albite     0.0  14.4
      K-Feldspar  0.0  7.8
      Fluorapatite  0.0  0.017
      Dolomite  0.0   Enstatite  21.7
      Yb2O3  0.0  0.0094
      Fe(OH)3  0.0  2.89
      Pyrite  0.0  0.17
      Zincite  0.0  Sphalerite  0.05
      Birnessite  0.0  0.008
      Barite  0.0  0.022
      Borax  0.0  0.07
      PuO2   0.0  8.76e-09
      CaUO4  0.0  0.000417
      Ca2V2O7  0.0  0.0035
      Tb2O3    0.0  0.03
      TcO2:2H2O(am)   0.0  5.72e-08
      Ca3(AsO4)2  0.0  0.0006
      Niter  0.0  0.001
      Halite    0.0  0.0009
      CaSeO4    0.0  1.8e-04
      O2(g)   -0.7   1.0
      CO2(g)    -3.5   1.0
      END
------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 3.     Solution after simulation 1.
Using pure phase assemblage 1.
Using reaction 1.

Reaction 1.     Irreversible reaction defined in simulation 2.

       1.000e+000 moles of the following reaction have been added:

                     Relative
      Reactant          moles


      NaCN                0.00
      NaI                 0.00

                     Relative
      Element           moles
      C                   0.00
```

```
      I                    0.00
      N                    0.00
      Na                   0.00

--------------------Phase assemblage--------------------------------

                                                        Moles in assemblage
Phase              SI log IAP  log KT    Initial      Final      Delta

Albite          -0.00    2.66    2.66 1.440e+001 1.418e+001-2.237e-001
Barite           0.00  -10.01  -10.01 2.200e-002 2.200e-002-1.923e-008
Birnessite       0.00  269.79  269.79 8.000e-003 8.000e-003-7.028e-014
Borax            0.00   12.04   12.04 7.000e-002 1.221e-002-5.779e-002
Ca2V2O7         -0.48   16.71   17.18 3.500e-003           -3.500e-003
Ca3(AsO4)2     -53.49  -35.69   17.80 6.000e-004           -6.000e-004
Calcite         -0.00    1.82    1.82 6.100e+000 5.975e+000-1.253e-001
CaSeO4          -4.28   -7.37   -3.09 1.800e-004           -1.800e-004
CaUO4           -0.00   15.94   15.94 4.170e-004 4.136e-004-3.407e-006
CO2(g)          -3.50  -11.33   -7.83 1.000e+000 1.063e+000 6.314e-002
Dolomite        -0.00    2.47    2.47
MgSiO3 is reactant     2.170e+001 2.272e+001 1.024e+000
Fe(OH)3          0.00   18.66   18.66 2.890e+000 3.060e+000 1.700e-001
Fluorapatite     0.00  -25.16  -25.16 1.700e-002 1.580e-002-1.200e-003
Gypsum          -0.00   -4.53   -4.53 1.300e-003 1.315e-001 1.302e-001
Halite          -5.40   -3.83    1.56 9.000e-004           -9.000e-004
Illite          -0.40    8.48    8.88 4.100e+000           -4.100e+000

K-Feldspar      -0.00   -0.38   -0.38 7.800e+000 1.026e+001 2.461e+000
Kaolinite        0.00    6.72    6.72 0.000e+000 3.597e+000 3.597e+000
Niter           -6.58   -6.81   -0.22 1.000e-003           -1.000e-003
O2(g)           -0.70   82.40   83.10 1.000e+000 3.618e-001-6.382e-001
PuO2             0.00  -25.93  -25.93 8.760e-009 8.760e-009-2.901e-013
Pyrite        -242.00 -325.69  -83.69 1.700e-001           -1.700e-001
Quartz           0.00   -4.03   -4.03 1.065e+002 1.059e+002-5.782e-001
Tb2O3           -7.09   40.01   47.10 3.000e-002           -3.000e-002
TcO2:2H2O(am)  -40.01  -77.23  -37.22 5.720e-008           -5.720e-008
Yb2O3           -9.39   38.41   47.80 9.400e-003           -9.400e-003
Zincite         -0.00   11.20   11.20
      ZnS is reactant    5.000e-002 4.988e-002-1.208e-004

-----------------Solution composition-----------------------------

      Elements           Molality       Moles

      Al                5.293e-008  4.972e-008
      As                1.277e-003  1.200e-003
      B                 2.460e-001  2.311e-001
      Ba                2.047e-008  1.923e-008
      C                 6.686e-002  6.281e-002
      Ca                1.094e-002  1.028e-002
      Cl                1.136e-003  1.067e-003
      F                 1.277e-003  1.200e-003
      Fe                4.660e-007  4.378e-007
```

I	1.010e-006	9.490e-007
K	3.562e-004	3.346e-004
Mg	9.261e-004	8.701e-004
Mn	6.060e-013	5.694e-013
N	1.294e-003	1.216e-003
Na	3.625e-001	3.405e-001
P	3.832e-003	3.600e-003
Pu	3.088e-013	2.901e-013
S	2.235e-001	2.100e-001
Se	1.916e-004	1.800e-004
Si	1.066e-004	1.002e-004
Tb	6.386e-002	6.000e-002
Tc	6.088e-008	5.720e-008
U	3.626e-006	3.407e-006
V	7.451e-003	7.000e-003
Yb	2.001e-002	1.880e-002
Zn	1.286e-004	1.208e-004

----------Description of solution----------

pH = 8.032 Charge balance
pe = 12.57 Adjusted to redox equilibrium

Activity of water	0.986
Ionic strength	5.454e-001
Mass of water (kg)	9.395e-001
Total alkalinity (eq/kg)	1.935e-001
Total CO2 (mol/kg)	6.686e-002
Temperature (deg C)	25.000
Electrical balance (eq)	2.197e-005
Percent error, 100*(Cat-|An|)/(Cat+|An|)	0.00
Iterations	44
Total H	1.049901e+002
Total O	5.392984e+001

----------Distribution of species----------

Species	Molality	Log Activity	Molality	Log Activity	Log Gamma
OH-	1.555e-006	1.023e-006	-5.808	-5.990	-0.182
H+	1.158e-008	9.281e-009	-7.936	-8.032	-0.096
H2O	5.553e+001	9.856e-001	-0.006	-0.006	0.000
Al	5.293e-008				
AlO2-	5.062e-008	3.429e-008	-7.296	-7.465	-0.169
NaAlO2	1.363e-009	1.363e-009	-8.866	-8.866	0.000
HAlO2	9.289e-010	9.289e-010	-9.032	-9.032	0.000
Al(OH)2+	8.747e-012	5.924e-012	-11.058	-11.227	-0.169
AlOH+2	1.203e-013	2.402e-014	-12.920	-13.619	-0.700
Al(SO4)2-	1.404e-015	9.508e-016	-14.853	-15.022	-0.169
AlSO4+	7.428e-016	5.031e-016	-15.129	-15.298	-0.169

Al+3	2.238e-016	2.019e-017	-15.650	-16.695	-1.045
AlHPO4+	1.197e-016	8.108e-017	-15.922	-16.091	-0.169
Al2(OH)2+4	3.447e-023	9.384e-026	-22.463	-25.028	-2.565
AlF+2	4.640e-024	9.267e-025	-23.334	-24.033	-0.700
AlH2PO4+2	1.888e-028	3.772e-029	-27.724	-28.423	-0.700
Al3(OH)4+5	9.127e-029	1.379e-032	-28.040	-31.860	-3.821
AlF2+	2.500e-033	1.693e-033	-32.602	-32.771	-0.169
AlF3	0.000e+000	0.000e+000	-43.009	-43.009	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-51.392	-58.902	-7.510
AlF4-	0.000e+000	0.000e+000	-54.778	-54.948	-0.169
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-185.600	-185.600	0.000
As(3)	0.000e+000				
HAsO2	0.000e+000	0.000e+000	-57.042	-57.042	0.000
As(OH)3	0.000e+000	0.000e+000	-57.107	-57.107	0.000
H2AsO3-	0.000e+000	0.000e+000	-58.118	-58.288	-0.169
AsO2-	0.000e+000	0.000e+000	-58.132	-58.301	-0.169
AsO2OH-2	0.000e+000	0.000e+000	-60.521	-61.265	-0.744
HAsS2	0.000e+000	0.000e+000	-333.373	-333.373	0.000
As(5)	1.277e-003				
AsO3F-2	1.275e-003	2.299e-004	-2.895	-3.639	-0.744
HAsO3F-	2.339e-006	1.584e-006	-5.631	-5.800	-0.169
HAsO4-2	2.785e-028	5.021e-029	-27.555	-28.299	-0.744
H2AsO4-	4.145e-030	2.807e-030	-29.382	-29.552	-0.169
AsO4-3	6.988e-031	1.388e-032	-30.156	-31.858	-1.702
H3AsO4	4.589e-036	4.589e-036	-35.338	-35.338	0.000
B(-5)	0.000e+000				
BH4-	0.000e+000	0.000e+000	-222.362	-222.531	-0.169
B(3)	2.460e-001				
B(OH)3	2.201e-001	2.201e-001	-0.657	-0.657	0.000
BO2-	1.905e-002	1.290e-002	-1.720	-1.889	-0.169
NaB(OH)4	5.169e-003	5.169e-003	-2.287	-2.287	0.000
CaB(OH)4+	1.624e-003	1.100e-003	-2.790	-2.959	-0.169
MgB(OH)4+	1.288e-004	8.725e-005	-3.890	-4.059	-0.169
BaB(OH)4+	2.177e-009	1.475e-009	-8.662	-8.831	-0.169
B2O(OH)5-	1.591e-012	1.077e-012	-11.798	-11.968	-0.169
BF2(OH)2-	2.671e-031	1.809e-031	-30.573	-30.743	-0.169
BF3OH-	0.000e+000	0.000e+000	-46.308	-46.477	-0.169
BF4-	0.000e+000	0.000e+000	-63.851	-64.020	-0.169
Ba	2.047e-008				
Ba+2	1.825e-008	3.993e-009	-7.739	-8.399	-0.660
BaB(OH)4+	2.177e-009	1.475e-009	-8.662	-8.831	-0.169
BaNO3+	3.832e-011	2.595e-011	-10.417	-10.586	-0.169
BaCO3	4.646e-012	4.646e-012	-11.333	-11.333	0.000
BaCl+	1.396e-012	9.457e-013	-11.855	-12.024	-0.169
BaOH+	2.121e-014	1.437e-014	-13.673	-13.843	-0.169
BaF+	1.864e-023	1.262e-023	-22.730	-22.899	-0.169
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-266.310	-266.310	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-238.631	-238.631	0.000

C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-148.248	-148.248	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-51.206	-51.206	0.000
C(4)	6.686e-002				
TbCO3+	2.686e-002	1.820e-002	-1.571	-1.740	-0.169
YbCO3+	9.874e-003	6.688e-003	-2.005	-2.175	-0.169
Tb(CO3)2-	9.716e-003	6.580e-003	-2.013	-2.182	-0.169
Yb(CO3)2-	4.867e-003	3.296e-003	-2.313	-2.482	-0.169
HCO3-	7.357e-004	4.983e-004	-3.133	-3.303	-0.169
NaHCO3	1.485e-004	1.485e-004	-3.828	-3.828	0.000
CO3-2	1.193e-005	2.382e-006	-4.924	-5.623	-0.700
TbHCO3+2	1.097e-005	2.191e-006	-4.960	-5.659	-0.700
CaHCO3+	1.084e-005	7.345e-006	-4.965	-5.134	-0.169
CO2	9.594e-006	1.088e-005	-5.018	-4.963	0.055
CaCO3	6.867e-006	6.867e-006	-5.163	-5.163	0.000
UO2(CO3)3-4	3.427e-006	3.103e-009	-5.465	-8.508	-3.043
NaCO3-	2.564e-006	1.736e-006	-5.591	-5.760	-0.169
YbHCO3+2	2.413e-006	4.819e-007	-5.618	-6.317	-0.700
MgHCO3+	7.087e-007	4.800e-007	-6.150	-6.319	-0.169
ZnCO3	2.765e-007	2.765e-007	-6.558	-6.558	0.000
ZnHCO3+	2.621e-007	1.775e-007	-6.582	-6.751	-0.169
MgCO3	2.090e-007	2.090e-007	-6.680	-6.680	0.000
UO2(CO3)2-2	1.606e-007	2.896e-008	-6.794	-7.538	-0.744
(UO2)2CO3(OH)3-	1.589e-009	1.076e-009	-8.799	-8.968	-0.169
UO2CO3	6.320e-010	6.320e-010	-9.199	-9.199	0.000
BaCO3	4.646e-012	4.646e-012	-11.333	-11.333	0.000
(UO2)3(CO3)6-6	2.592e-013	3.457e-020	-12.586	-19.461	-6.875
PuO2(CO3)2-2	2.396e-013	4.320e-014	-12.620	-13.364	-0.744
FeCO3+	7.391e-015	5.006e-015	-14.131	-14.301	-0.169
MnCO3	4.895e-015	4.895e-015	-14.310	-14.310	0.000
MnHCO3+	3.288e-016	2.227e-016	-15.483	-15.652	-0.169
FeHCO3+	3.931e-019	2.663e-019	-18.405	-18.575	-0.169
FeCO3	1.377e-019	1.377e-019	-18.861	-18.861	0.000
(UO2)3(OH)5CO2+	3.324e-021	2.251e-021	-20.478	-20.648	-0.169
(UO2)3O(OH)2(HCO3)+	2.719e-021	1.842e-021	-20.566	-20.735	-0.169
UO2(CO3)3-5	9.239e-030	1.578e-034	-29.034	-33.802	-4.767
U(CO3)4-4	0.000e+000	0.000e+000	-45.777	-48.820	-3.043
(UO2)11(CO3)6(OH)12-2	0.000e+000	0.000e+000	-46.342	-47.086	-0.744
U(CO3)5-6	0.000e+000	0.000e+000	-48.651	-55.526	-6.875
SCN-	0.000e+000	0.000e+000	-214.854	-215.036	-0.182
UO2SCN+	0.000e+000	0.000e+000	-226.733	-226.902	-0.169
USCN+3	0.000e+000	0.000e+000	-272.031	-273.544	-1.513
Zn(SCN)2	0.000e+000	0.000e+000	-434.051	-434.051	0.000
UO2(SCN)2	0.000e+000	0.000e+000	-442.106	-442.106	0.000
U(SCN)2+2	0.000e+000	0.000e+000	-486.579	-487.279	-0.700
UO2(SCN)3-	0.000e+000	0.000e+000	-656.113	-656.282	-0.169
Zn(SCN)4-2	0.000e+000	0.000e+000	-863.012	-863.756	-0.744
Ca	1.094e-002				
Ca+2	4.868e-003	1.244e-003	-2.313	-2.905	-0.593
CaSO4	4.424e-003	4.424e-003	-2.354	-2.354	0.000
CaB(OH)4+	1.624e-003	1.100e-003	-2.790	-2.959	-0.169

CaHCO3+	1.084e-005	7.345e-006	-4.965	-5.134	-0.169
CaNO3+	7.533e-006	5.102e-006	-5.123	-5.292	-0.169
CaCO3	6.867e-006	6.867e-006	-5.163	-5.163	0.000
CaCl+	2.749e-007	1.862e-007	-6.561	-6.730	-0.169
CaHPO4	1.093e-007	1.093e-007	-6.961	-6.961	0.000
CaPO4-	4.349e-008	2.946e-008	-7.362	-7.531	-0.169
CaOH+	2.755e-008	1.866e-008	-7.560	-7.729	-0.169
CaCl2	1.546e-010	1.546e-010	-9.811	-9.811	0.000
CaP2O7-2	2.025e-013	3.650e-014	-12.694	-13.438	-0.744
CaH2PO4+	6.845e-017	4.636e-017	-16.165	-16.334	-0.169
CaF+	4.285e-017	2.902e-017	-16.368	-16.537	-0.169
Cl(-1)	1.136e-003				
Cl-	1.109e-003	7.061e-004	-2.955	-3.151	-0.196
NaCl	2.585e-005	2.585e-005	-4.587	-4.587	0.000
TbCl+2	5.296e-007	1.058e-007	-6.276	-6.976	-0.700
CaCl+	2.749e-007	1.862e-007	-6.561	-6.730	-0.169
YbCl+2	7.096e-008	1.417e-008	-7.149	-7.849	-0.700
MgCl+	6.751e-008	4.572e-008	-7.171	-7.340	-0.169
Zn(OH)Cl	2.977e-008	2.977e-008	-7.526	-7.526	0.000
ZnCl+	2.421e-008	1.640e-008	-7.616	-7.785	-0.169
KCl	4.538e-009	4.538e-009	-8.343	-8.343	0.000
CaCl2	1.546e-010	1.546e-010	-9.811	-9.811	0.000
TbCl2+	6.037e-011	4.089e-011	-10.219	-10.388	-0.169
ZnCl2	1.352e-011	1.352e-011	-10.869	-10.869	0.000
YbCl2+	5.854e-012	3.965e-012	-11.233	-11.402	-0.169
HCl	1.472e-012	1.472e-012	-11.832	-11.832	0.000
BaCl+	1.396e-012	9.457e-013	-11.855	-12.024	-0.169
TbCl3	1.132e-014	1.132e-014	-13.946	-13.946	0.000
ZnCl3-	7.785e-015	5.273e-015	-14.109	-14.278	-0.169
YbCl3	8.967e-016	8.967e-016	-15.047	-15.047	0.000
ZnCl4-2	1.565e-016	2.822e-017	-15.805	-16.549	-0.744
MnCl+	1.303e-016	8.826e-017	-15.885	-16.054	-0.169
UO2Cl+	8.201e-017	5.554e-017	-16.086	-16.255	-0.169
TbCl4-	4.334e-018	2.935e-018	-17.363	-17.532	-0.169
YbCl4-	3.463e-019	2.345e-019	-18.461	-18.630	-0.169
PuO2Cl+	5.367e-021	3.635e-021	-20.270	-20.439	-0.169
UO2Cl2	2.008e-021	2.008e-021	-20.697	-20.697	0.000
FeCl+	7.733e-022	5.237e-022	-21.112	-21.281	-0.169
FeCl+2	2.143e-022	4.281e-023	-21.669	-22.368	-0.700
FeCl2+	3.613e-023	2.447e-023	-22.442	-22.611	-0.169
MnCl3-	1.419e-023	9.611e-024	-22.848	-23.017	-0.169
FeCl2	1.984e-027	1.984e-027	-26.702	-26.702	0.000
FeCl4-	2.165e-032	1.467e-032	-31.664	-31.834	-0.169
FeCl4-2	1.585e-032	2.858e-033	-31.800	-32.544	-0.744
UCl+3	0.000e+000	0.000e+000	-61.407	-62.920	-1.513
Cl(1)	1.592e-020				
ClO-	1.291e-020	8.744e-021	-19.889	-20.058	-0.169
HClO	3.009e-021	3.009e-021	-20.522	-20.522	0.000
Cl(3)	2.038e-030				
ClO2-	2.038e-030	1.380e-030	-29.691	-29.860	-0.169
HClO2	1.894e-035	1.894e-035	-34.723	-34.723	0.000

Cl(5)	2.357e-026				
ClO3-	2.357e-026	1.550e-026	-25.628	-25.810	-0.182
UO2ClO3+	3.880e-039	2.628e-039	-38.411	-38.580	-0.169
Cl(7)	1.322e-026				
ClO4-	1.321e-026	8.694e-027	-25.879	-26.061	-0.182
ZnClO4+	3.356e-030	2.273e-030	-29.474	-29.643	-0.169
F	1.277e-003				
AsO3F-2	1.275e-003	2.299e-004	-2.895	-3.639	-0.744
HAsO3F-	2.339e-006	1.584e-006	-5.631	-5.800	-0.169
TbF+2	9.275e-014	1.852e-014	-13.033	-13.732	-0.700
YbF+2	2.065e-014	4.124e-015	-13.685	-14.385	-0.700
F-	6.976e-015	4.590e-015	-14.156	-14.338	-0.182
NaF	1.023e-016	1.023e-016	-15.990	-15.990	0.000
CaF+	4.285e-017	2.902e-017	-16.368	-16.537	-0.169
MgF+	1.357e-017	9.188e-018	-16.868	-17.037	-0.169
ZnF+	1.323e-018	8.961e-019	-17.878	-18.048	-0.169
HF	6.539e-020	6.539e-020	-19.184	-19.184	0.000
PO3F-2	6.064e-022	1.093e-022	-21.217	-21.961	-0.744
UO2F+	4.224e-023	2.861e-023	-22.374	-22.543	-0.169
BaF+	1.864e-023	1.262e-023	-22.730	-22.899	-0.169
AlF+2	4.640e-024	9.267e-025	-23.334	-24.033	-0.700
VO2F	1.523e-024	1.523e-024	-23.817	-23.817	0.000
TbF2+	4.048e-025	2.742e-025	-24.393	-24.562	-0.169
YbF2+	1.073e-025	7.270e-026	-24.969	-25.138	-0.169
PuO2F+	2.660e-026	1.802e-026	-25.575	-25.744	-0.169
HPO3F-	1.884e-026	1.276e-026	-25.725	-25.894	-0.169
MnF+	1.071e-026	7.252e-027	-25.970	-26.140	-0.169
FeF+2	1.254e-028	2.505e-029	-27.902	-28.601	-0.700
BF2(OH)2-	2.671e-031	1.809e-031	-30.573	-30.743	-0.169
FeF+	1.581e-031	1.071e-031	-30.801	-30.970	-0.169
AlF2+	2.500e-033	1.693e-033	-32.602	-32.771	-0.169
H2PO3F	7.574e-034	7.574e-034	-33.121	-33.121	0.000
UO2F2	3.941e-034	3.941e-034	-33.404	-33.404	0.000
HF2-	1.073e-034	7.270e-035	-33.969	-34.138	-0.169
VOF+	1.935e-035	1.310e-035	-34.713	-34.883	-0.169
PuO2F2	1.634e-035	1.634e-035	-34.787	-34.787	0.000
VO2F2-	2.977e-036	2.016e-036	-35.526	-35.696	-0.169
TbF3	4.612e-037	4.612e-037	-36.336	-36.336	0.000
YbF3	1.657e-037	1.657e-037	-36.781	-36.781	0.000
H2F2	1.064e-038	1.064e-038	-37.973	-37.973	0.000
FeF2+	2.747e-039	1.860e-039	-38.561	-38.730	-0.169
AlF3	0.000e+000	0.000e+000	-43.009	-43.009	0.000
PuF+3	0.000e+000	0.000e+000	-43.844	-45.356	-1.513
PuO2F3-	0.000e+000	0.000e+000	-43.990	-44.159	-0.169
UO2F3-	0.000e+000	0.000e+000	-45.307	-45.476	-0.169
BF3OH-	0.000e+000	0.000e+000	-46.308	-46.477	-0.169
VOF2	0.000e+000	0.000e+000	-46.441	-46.441	0.000
TbF4-	0.000e+000	0.000e+000	-48.429	-48.598	-0.169
YbF4-	0.000e+000	0.000e+000	-48.777	-48.946	-0.169
PuF2+2	0.000e+000	0.000e+000	-52.055	-52.755	-0.700
AlF4-	0.000e+000	0.000e+000	-54.778	-54.948	-0.169

PuO2F4-2	0.000e+000	0.000e+000	-54.880	-55.624	-0.744
UO2F4-2	0.000e+000	0.000e+000	-58.295	-59.039	-0.744
BF4-	0.000e+000	0.000e+000	-63.851	-64.020	-0.169
UF+3	0.000e+000	0.000e+000	-65.050	-66.563	-1.513
UF2+2	0.000e+000	0.000e+000	-73.275	-73.975	-0.700
PuF3+	0.000e+000	0.000e+000	-77.024	-77.193	-0.169
UF3+	0.000e+000	0.000e+000	-82.792	-82.962	-0.169
PuF4	0.000e+000	0.000e+000	-92.631	-92.631	0.000
UF4	0.000e+000	0.000e+000	-93.356	-93.356	0.000
SiF6-2	0.000e+000	0.000e+000	-95.043	-95.787	-0.744
UF5-	0.000e+000	0.000e+000	-106.197	-106.366	-0.169
UF6-2	0.000e+000	0.000e+000	-117.930	-118.674	-0.744
Fe(2)	8.497e-018				
Fe+2	3.984e-018	1.018e-018	-17.400	-17.992	-0.593
FeSO4	3.929e-018	3.929e-018	-17.406	-17.406	0.000
FeHCO3+	3.931e-019	2.663e-019	-18.405	-18.575	-0.169
FeCO3	1.377e-019	1.377e-019	-18.861	-18.861	0.000
FeOH+	5.049e-020	3.419e-020	-19.297	-19.466	-0.169
FePO4-	1.051e-021	7.115e-022	-20.979	-21.148	-0.169
FeCl+	7.733e-022	5.237e-022	-21.112	-21.281	-0.169
FeHPO4	6.480e-022	6.480e-022	-21.188	-21.188	0.000
Fe(OH)2	2.885e-023	2.885e-023	-22.540	-22.540	0.000
Fe(OH)3-	1.801e-025	1.220e-025	-24.745	-24.914	-0.169
FeCl2	1.984e-027	1.984e-027	-26.702	-26.702	0.000
FeH2PO4+	1.118e-030	7.571e-031	-29.952	-30.121	-0.169
FeF+	1.581e-031	1.071e-031	-30.801	-30.970	-0.169
Fe(OH)4-2	7.183e-032	1.295e-032	-31.144	-31.888	-0.744
FeCl4-2	1.585e-032	2.858e-033	-31.800	-32.544	-0.744
Fe(3)	4.660e-007				
Fe(OH)3	4.359e-007	4.359e-007	-6.361	-6.361	0.000
Fe(OH)4-	1.717e-008	1.163e-008	-7.765	-7.935	-0.169
Fe(OH)2+	1.296e-008	8.774e-009	-7.888	-8.057	-0.169
FeOH+2	1.249e-012	2.495e-013	-11.903	-12.603	-0.700
FeCO3+	7.391e-015	5.006e-015	-14.131	-14.301	-0.169
FeHPO4+	1.300e-015	8.805e-016	-14.886	-15.055	-0.169
Fe+3	4.033e-018	3.639e-019	-17.394	-18.439	-1.045
FeSO4+	1.266e-018	8.572e-019	-17.898	-18.067	-0.169
Fe(SO4)2-	5.210e-019	3.529e-019	-18.283	-18.452	-0.169
FeNO3+2	1.491e-020	2.978e-021	-19.827	-20.526	-0.700
Fe2(OH)2+4	6.154e-022	1.676e-024	-21.211	-23.776	-2.565
FeCl+2	2.143e-022	4.281e-023	-21.669	-22.368	-0.700
FeCl2+	3.613e-023	2.447e-023	-22.442	-22.611	-0.169
Fe3(OH)4+5	2.032e-026	3.072e-030	-25.692	-29.513	-3.821
FeF+2	1.254e-028	2.505e-029	-27.902	-28.601	-0.700
FeH2PO4+2	3.998e-029	7.986e-030	-28.398	-29.098	-0.700
FeNO2+2	7.702e-032	1.538e-032	-31.113	-31.813	-0.700
FeCl4-	2.165e-032	1.467e-032	-31.664	-31.834	-0.169
FeF2+	2.747e-039	1.860e-039	-38.561	-38.730	-0.169
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-44.363	-44.308	0.055

I(-03)	0.000e+000				
I3-	0.000e+000	0.000e+000	-48.263	-48.432	-0.169
I(-1)	5.662e-019				
I-	5.639e-019	3.590e-019	-18.249	-18.445	-0.196
NaI	2.251e-021	2.251e-021	-20.648	-20.648	0.000
KI	1.776e-024	1.776e-024	-23.751	-23.751	0.000
ZnI+	7.103e-027	4.811e-027	-26.149	-26.318	-0.169
ZnI2	0.000e+000	0.000e+000	-43.593	-43.593	0.000
ZnI3-	0.000e+000	0.000e+000	-62.030	-62.200	-0.169
UI+3	0.000e+000	0.000e+000	-77.203	-78.716	-1.513
ZnI4-2	0.000e+000	0.000e+000	-80.500	-81.244	-0.744
I(1)	1.033e-021				
IO-	1.033e-021	6.996e-022	-20.986	-21.155	-0.169
I(5)	1.010e-006				
IO3-	1.010e-006	6.841e-007	-5.996	-6.165	-0.169
HIO3	1.969e-014	1.969e-014	-13.706	-13.706	0.000
UO2IO3+	2.824e-018	1.913e-018	-17.549	-17.718	-0.169
UO2(IO3)2	2.457e-023	2.457e-023	-22.610	-22.610	0.000
I(7)	3.191e-019				
IO4-	3.191e-019	2.100e-019	-18.496	-18.678	-0.182
K	3.562e-004				
K+	3.006e-004	1.914e-004	-3.522	-3.718	-0.196
KSO4-	5.553e-005	3.761e-005	-4.255	-4.425	-0.169
KCl	4.538e-009	4.538e-009	-8.343	-8.343	0.000
KHPO4-	2.722e-010	1.844e-010	-9.565	-9.734	-0.169
KOH	7.047e-011	7.047e-011	-10.152	-10.152	0.000
KHSO4	3.080e-013	3.080e-013	-12.511	-12.511	0.000
KP2O7-3	1.065e-017	2.116e-019	-16.973	-18.674	-1.702
KI	1.776e-024	1.776e-024	-23.751	-23.751	0.000
Mg	9.261e-004				
MgSO4	5.393e-004	5.393e-004	-3.268	-3.268	0.000
Mg+2	2.569e-004	8.294e-005	-3.590	-4.081	-0.491
MgB(OH)4+	1.288e-004	8.725e-005	-3.890	-4.059	-0.169
MgHCO3+	7.087e-007	4.800e-007	-6.150	-6.319	-0.169
MgCO3	2.090e-007	2.090e-007	-6.680	-6.680	0.000
MgCl+	6.751e-008	4.572e-008	-7.171	-7.340	-0.169
MgHPO4	1.078e-008	1.078e-008	-7.967	-7.967	0.000
MgPO4-	3.903e-009	2.643e-009	-8.409	-8.578	-0.169
MgP2O7-2	3.997e-014	7.207e-015	-13.398	-14.142	-0.744
MgF+	1.357e-017	9.188e-018	-16.868	-17.037	-0.169
MgH2PO4+	8.306e-018	5.625e-018	-17.081	-17.250	-0.169
Mg4(OH)4+4	3.933e-022	1.071e-024	-21.405	-23.970	-2.565
Mn(2)	5.887e-013				
MnSO4	3.527e-013	3.527e-013	-12.453	-12.453	0.000
Mn+2	2.297e-013	5.870e-014	-12.639	-13.231	-0.593
MnCO3	4.895e-015	4.895e-015	-14.310	-14.310	0.000
MnSeO4	5.456e-016	5.456e-016	-15.263	-15.263	0.000
MnHCO3+	3.288e-016	2.227e-016	-15.483	-15.652	-0.169
MnOH+	2.366e-016	1.603e-016	-15.626	-15.795	-0.169
MnCl+	1.303e-016	8.826e-017	-15.885	-16.054	-0.169
MnNO3+	1.124e-016	7.614e-017	-15.949	-16.118	-0.169

MnHPO4	3.568e-017	3.568e-017	-16.448	-16.448	0.000
MnPO4-	1.102e-017	7.465e-018	-16.958	-17.127	-0.169
Mn(NO3)2	1.565e-019	1.565e-019	-18.805	-18.805	0.000
MnH2PO4+	4.620e-020	3.129e-020	-19.335	-19.505	-0.169
Mn(OH)2	4.178e-020	4.178e-020	-19.379	-19.379	0.000
MnCl3-	1.419e-023	9.611e-024	-22.848	-23.017	-0.169
Mn(OH)3-	6.144e-024	4.162e-024	-23.212	-23.381	-0.169
MnF+	1.071e-026	7.252e-027	-25.970	-26.140	-0.169
Mn2(OH)3+	7.673e-027	5.197e-027	-26.115	-26.284	-0.169
Mn2OH+3	3.283e-028	1.008e-029	-27.484	-28.997	-1.513
Mn(OH)4-2	2.076e-029	3.743e-030	-28.683	-29.427	-0.744
Mn(3)	1.901e-025				
Mn+3	1.901e-025	5.836e-027	-24.721	-26.234	-1.513
Mn(6)	3.851e-017				
MnO4-2	3.851e-017	6.943e-018	-16.414	-17.158	-0.744
Mn(7)	1.732e-014				
MnO4-	1.732e-014	1.140e-014	-13.761	-13.943	-0.182
N(-03)	0.000e+000				
N3-	0.000e+000	0.000e+000	-100.039	-100.208	-0.169
HN3	0.000e+000	0.000e+000	-103.538	-103.538	0.000
ZnN3+	0.000e+000	0.000e+000	-104.456	-104.625	-0.169
UO2N3+	0.000e+000	0.000e+000	-110.736	-110.905	-0.169
Zn(N3)2	0.000e+000	0.000e+000	-204.080	-204.080	0.000
UO2(N3)2	0.000e+000	0.000e+000	-209.363	-209.363	0.000
UO2(N3)3-	0.000e+000	0.000e+000	-307.991	-308.161	-0.169
UO2(N3)4-2	0.000e+000	0.000e+000	-408.445	-409.189	-0.744
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-64.589	-64.802	-0.213
NH3	0.000e+000	0.000e+000	-66.009	-66.009	0.000
Zn(NH3)+2	0.000e+000	0.000e+000	-68.116	-68.816	-0.700
NH4SO4-	0.000e+000	0.000e+000	-74.546	-74.715	-0.169
Zn(NH3)2+2	0.000e+000	0.000e+000	-131.919	-132.619	-0.700
Zn(NH3)3+2	0.000e+000	0.000e+000	-195.722	-196.421	-0.700
SCN-	0.000e+000	0.000e+000	-214.854	-215.036	-0.182
UO2SCN+	0.000e+000	0.000e+000	-226.733	-226.902	-0.169
Zn(NH3)4+2	0.000e+000	0.000e+000	-259.798	-260.498	-0.700
USCN+3	0.000e+000	0.000e+000	-272.031	-273.544	-1.513
Zn(SCN)2	0.000e+000	0.000e+000	-434.051	-434.051	0.000
UO2(SCN)2	0.000e+000	0.000e+000	-442.106	-442.106	0.000
U(SCN)2+2	0.000e+000	0.000e+000	-486.579	-487.279	-0.700
UO2(SCN)3-	0.000e+000	0.000e+000	-656.113	-656.282	-0.169
Zn(SCN)4-2	0.000e+000	0.000e+000	-863.012	-863.756	-0.744
N(-5)	0.000e+000				
HCN	0.000e+000	0.000e+000	-122.324	-122.324	0.000
CN-	0.000e+000	0.000e+000	-123.354	-123.550	-0.196
Zn(CN)4-2	0.000e+000	0.000e+000	-481.542	-482.286	-0.744
N(0)	2.354e-021				
N2	1.177e-021	1.177e-021	-20.929	-20.929	0.000
N(3)	4.702e-017				
NO2-	4.702e-017	2.993e-017	-16.328	-16.524	-0.196
HNO2	4.741e-022	4.741e-022	-21.324	-21.324	0.000

FeNO2+2	7.702e-032	1.538e-032	-31.113	-31.813	-0.700
N(5)	1.294e-003				
NO3-	1.285e-003	8.183e-004	-2.891	-3.087	-0.196
CaNO3+	7.533e-006	5.102e-006	-5.123	-5.292	-0.169
TbNO3+2	1.157e-006	2.312e-007	-5.937	-6.636	-0.700
YbNO3+2	9.307e-008	1.859e-008	-7.031	-7.731	-0.700
BaNO3+	3.832e-011	2.595e-011	-10.417	-10.586	-0.169
HNO3	3.972e-013	3.972e-013	-12.401	-12.401	0.000
UO2NO3+	1.219e-016	8.255e-017	-15.914	-16.083	-0.169
MnNO3+	1.124e-016	7.614e-017	-15.949	-16.118	-0.169
Mn(NO3)2	1.565e-019	1.565e-019	-18.805	-18.805	0.000
FeNO3+2	1.491e-020	2.978e-021	-19.827	-20.526	-0.700
UNO3+3	0.000e+000	0.000e+000	-61.610	-63.123	-1.513
U(NO3)2+2	0.000e+000	0.000e+000	-64.700	-65.400	-0.700
Na	3.625e-001				
Na+	3.076e-001	2.083e-001	-0.512	-0.681	-0.169
NaSO4-	4.949e-002	3.352e-002	-1.306	-1.475	-0.169
NaB(OH)4	5.169e-003	5.169e-003	-2.287	-2.287	0.000
NaHCO3	1.485e-004	1.485e-004	-3.828	-3.828	0.000
NaCl	2.585e-005	2.585e-005	-4.587	-4.587	0.000
NaHSiO3	1.117e-005	1.117e-005	-4.952	-4.952	0.000
NaCO3-	2.564e-006	1.736e-006	-5.591	-5.760	-0.169
NaHPO4-	4.091e-007	2.771e-007	-6.388	-6.557	-0.169
NaOH	3.678e-008	3.678e-008	-7.434	-7.434	0.000
NaAlO2	1.363e-009	1.363e-009	-8.866	-8.866	0.000
Na2P2O7-2	1.734e-014	3.127e-015	-13.761	-14.505	-0.744
NaP2O7-3	9.512e-015	1.889e-016	-14.022	-15.724	-1.702
NaHP2O7-2	1.968e-015	3.548e-016	-14.706	-15.450	-0.744
NaF	1.023e-016	1.023e-016	-15.990	-15.990	0.000
NaI	2.251e-021	2.251e-021	-20.648	-20.648	0.000
O(0)	4.507e-004				
O2	2.254e-004	2.556e-004	-3.647	-3.592	0.055
UO2S2O3	0.000e+000	0.000e+000	-156.680	-156.680	0.000
S3O6-2	0.000e+000	0.000e+000	-175.021	-175.765	-0.744
S2-2	0.000e+000	0.000e+000	-249.276	-250.020	-0.744
S4O6-2	0.000e+000	0.000e+000	-266.022	-266.766	-0.744
S3-2	0.000e+000	0.000e+000	-353.700	-354.444	-0.744
S5O6-2	0.000e+000	0.000e+000	-385.902	-386.646	-0.744
S4-2	0.000e+000	0.000e+000	-458.351	-459.095	-0.744
S5-2	0.000e+000	0.000e+000	-563.218	-563.962	-0.744
P(-3)	0.000e+000				
PH4+	0.000e+000	0.000e+000	-236.280	-236.450	-0.169
P(5)	3.832e-003				
TbPO4	1.700e-003	1.700e-003	-2.770	-2.770	0.000
YbPO4	8.515e-004	8.515e-004	-3.070	-3.070	0.000
Yb(PO4)2-3	3.519e-004	6.990e-006	-3.454	-5.156	-1.702
Tb(PO4)2-3	2.797e-004	5.556e-006	-3.553	-5.255	-1.702
TbHPO4+	1.228e-005	8.315e-006	-4.911	-5.080	-0.169
YbHPO4+	3.082e-006	2.087e-006	-5.511	-5.680	-0.169
HPO4-2	8.867e-007	1.599e-007	-6.052	-6.796	-0.744
NaHPO4-	4.091e-007	2.771e-007	-6.388	-6.557	-0.169

CaHPO4	1.093e-007	1.093e-007	-6.961	-6.961	0.000
CaPO4-	4.349e-008	2.946e-008	-7.362	-7.531	-0.169
H2PO4-	3.705e-008	2.509e-008	-7.431	-7.600	-0.169
ZnPO4-	1.755e-008	1.188e-008	-7.756	-7.925	-0.169
Tb(HPO4)2-	1.559e-008	1.056e-008	-7.807	-7.976	-0.169
MgHPO4	1.078e-008	1.078e-008	-7.967	-7.967	0.000
Yb(HPO4)2-	7.809e-009	5.289e-009	-8.107	-8.277	-0.169
ZnHPO4	4.021e-009	4.021e-009	-8.396	-8.396	0.000
MgPO4-	3.903e-009	2.643e-009	-8.409	-8.578	-0.169
TbH2PO4+2	1.628e-009	3.252e-010	-8.788	-9.488	-0.700
PO4-3	3.931e-010	7.807e-012	-9.406	-11.107	-1.702
YbH2PO4+2	3.591e-010	7.172e-011	-9.445	-10.144	-0.700
KHPO4-	2.722e-010	1.844e-010	-9.565	-9.734	-0.169
UO2PO4-	1.616e-010	1.095e-010	-9.792	-9.961	-0.169
UO2HPO4	2.327e-012	2.327e-012	-11.633	-11.633	0.000
CaP2O7-2	2.025e-013	3.650e-014	-12.694	-13.438	-0.744
MgP2O7-2	3.997e-014	7.207e-015	-13.398	-14.142	-0.744
H3PO4	3.588e-014	3.588e-014	-13.445	-13.445	0.000
VO2HPO4-	2.365e-014	1.602e-014	-13.626	-13.795	-0.169
Na2P2O7-2	1.734e-014	3.127e-015	-13.761	-14.505	-0.744
NaP2O7-3	9.512e-015	1.889e-016	-14.022	-15.724	-1.702
P2O7-4	5.559e-015	5.034e-018	-14.255	-17.298	-3.043
HP2O7-3	3.839e-015	7.626e-017	-14.416	-16.118	-1.702
NaHP2O7-2	1.968e-015	3.548e-016	-14.706	-15.450	-0.744
FeHPO4+	1.300e-015	8.805e-016	-14.886	-15.055	-0.169
AlHPO4+	1.197e-016	8.108e-017	-15.922	-16.091	-0.169
VO2(HPO4)2-3	7.593e-017	1.508e-018	-16.120	-17.822	-1.702
CaH2PO4+	6.845e-017	4.636e-017	-16.165	-16.334	-0.169
UO2H2PO4+	5.442e-017	3.686e-017	-16.264	-16.433	-0.169
MnHPO4	3.568e-017	3.568e-017	-16.448	-16.448	0.000
H2P2O7-2	1.624e-017	2.927e-018	-16.790	-17.534	-0.744
MnPO4-	1.102e-017	7.465e-018	-16.958	-17.127	-0.169
KP2O7-3	1.065e-017	2.116e-019	-16.973	-18.674	-1.702
MgH2PO4+	8.306e-018	5.625e-018	-17.081	-17.250	-0.169
ZnH2PO4+	8.149e-020	5.519e-020	-19.089	-19.258	-0.169
MnH2PO4+	4.620e-020	3.129e-020	-19.335	-19.505	-0.169
Pu(HPO4)4-4	5.760e-021	5.216e-024	-20.240	-23.283	-3.043
PuO2H2PO4+	3.108e-021	2.105e-021	-20.508	-20.677	-0.169
FePO4-	1.051e-021	7.115e-022	-20.979	-21.148	-0.169
FeHPO4	6.480e-022	6.480e-022	-21.188	-21.188	0.000
UO2(H2PO4)2	6.452e-022	6.452e-022	-21.190	-21.190	0.000
PO3F-2	6.064e-022	1.093e-022	-21.217	-21.961	-0.744
H3P2O7-	9.219e-024	6.244e-024	-23.035	-23.205	-0.169
UO2H3PO4+2	7.476e-025	1.493e-025	-24.126	-24.826	-0.700
Pu(HPO4)3-2	2.646e-026	4.770e-027	-25.577	-26.321	-0.744
HPO3F-	1.884e-026	1.276e-026	-25.725	-25.894	-0.169
VO2H2PO4	1.053e-026	1.053e-026	-25.978	-25.978	0.000
AlH2PO4+2	1.888e-028	3.772e-029	-27.724	-28.423	-0.700
UO2(H2PO4)(H3PO4)+	9.047e-029	6.127e-029	-28.043	-28.213	-0.169
FeH2PO4+2	3.998e-029	7.986e-030	-28.398	-29.098	-0.700
Pu(HPO4)2	6.556e-030	6.556e-030	-29.183	-29.183	0.000

H4P2O7	1.703e-030	1.703e-030	-29.769	-29.769	0.000
FeH2PO4+	1.118e-030	7.571e-031	-29.952	-30.121	-0.169
PuHPO4+2	2.968e-033	5.929e-034	-32.527	-33.227	-0.700
H2PO3F	7.574e-034	7.574e-034	-33.121	-33.121	0.000
PuH2PO4+2	3.472e-040	0.000e+000	-39.459	-40.159	-0.700
Pu(3)	1.752e-032				
Pu(SO4)2-	1.612e-032	1.092e-032	-31.793	-31.962	-0.169
PuSO4+	1.062e-033	7.192e-034	-32.974	-33.143	-0.169
Pu+3	2.871e-034	8.816e-036	-33.542	-35.055	-1.513
PuOH+2	5.022e-035	1.003e-035	-34.299	-34.999	-0.700
PuH2PO4+2	3.472e-040	0.000e+000	-39.459	-40.159	-0.700
Pu(4)	1.376e-017				
Pu(OH)4	1.375e-017	1.375e-017	-16.862	-16.862	0.000
Pu(HPO4)4-4	5.760e-021	5.216e-024	-20.240	-23.283	-3.043
Pu(OH)3+	3.020e-021	2.046e-021	-20.520	-20.689	-0.169
Pu(OH)2+2	8.891e-026	1.776e-026	-25.051	-25.751	-0.700
Pu(HPO4)3-2	2.646e-026	4.770e-027	-25.577	-26.321	-0.744
Pu(HPO4)2	6.556e-030	6.556e-030	-29.183	-29.183	0.000
PuOH+3	3.603e-031	1.106e-032	-30.443	-31.956	-1.513
Pu(SO4)2	3.730e-033	3.730e-033	-32.428	-32.428	0.000
PuHPO4+2	2.968e-033	5.929e-034	-32.527	-33.227	-0.700
PuSO4+2	2.596e-035	5.186e-036	-34.586	-35.285	-0.700
Pu+4	1.221e-037	3.325e-040	-36.913	-39.478	-2.565
PuF+3	0.000e+000	0.000e+000	-43.844	-45.356	-1.513
PuF2+2	0.000e+000	0.000e+000	-52.055	-52.755	-0.700
PuF3+	0.000e+000	0.000e+000	-77.024	-77.193	-0.169
PuF4	0.000e+000	0.000e+000	-92.631	-92.631	0.000
Pu(5)	6.585e-014				
PuO2+	6.483e-014	4.391e-014	-13.188	-13.357	-0.169
PuO2OH	1.021e-015	1.021e-015	-14.991	-14.991	0.000
Pu(6)	2.429e-013				
PuO2(CO3)2-2	2.396e-013	4.320e-014	-12.620	-13.364	-0.744
PuO2OH+	2.901e-015	1.965e-015	-14.537	-14.707	-0.169
PuO2SO4	3.719e-016	3.719e-016	-15.430	-15.430	0.000
PuO2+2	4.035e-017	8.060e-018	-16.394	-17.094	-0.700
PuO2Cl+	5.367e-021	3.635e-021	-20.270	-20.439	-0.169
PuO2H2PO4+	3.108e-021	2.105e-021	-20.508	-20.677	-0.169
PuO2F+	2.660e-026	1.802e-026	-25.575	-25.744	-0.169
(PuO2)2(OH)2+2	2.011e-026	4.016e-027	-25.697	-26.396	-0.700
(PuO2)3(OH)5+	2.295e-033	1.555e-033	-32.639	-32.808	-0.169
PuO2F2	1.634e-035	1.634e-035	-34.787	-34.787	0.000
PuO2F3-	0.000e+000	0.000e+000	-43.990	-44.159	-0.169
PuO2F4-2	0.000e+000	0.000e+000	-54.880	-55.624	-0.744
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-140.562	-140.744	-0.182
H2S	0.000e+000	0.000e+000	-141.767	-141.767	0.000
S-2	0.000e+000	0.000e+000	-144.977	-145.637	-0.660
SCN-	0.000e+000	0.000e+000	-214.854	-215.036	-0.182
UO2SCN+	0.000e+000	0.000e+000	-226.733	-226.902	-0.169
S2-2	0.000e+000	0.000e+000	-249.276	-250.020	-0.744
USCN+3	0.000e+000	0.000e+000	-272.031	-273.544	-1.513

HAsS2	0.000e+000	0.000e+000	-333.373	-333.373	0.000
S3-2	0.000e+000	0.000e+000	-353.700	-354.444	-0.744
Zn(SCN)2	0.000e+000	0.000e+000	-434.051	-434.051	0.000
UO2(SCN)2	0.000e+000	0.000e+000	-442.106	-442.106	0.000
S4-2	0.000e+000	0.000e+000	-458.351	-459.095	-0.744
U(SCN)2+2	0.000e+000	0.000e+000	-486.579	-487.279	-0.700
S5-2	0.000e+000	0.000e+000	-563.218	-563.962	-0.744
UO2(SCN)3-	0.000e+000	0.000e+000	-656.113	-656.282	-0.169
Zn(SCN)4-2	0.000e+000	0.000e+000	-863.012	-863.756	-0.744
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-144.831	-145.575	-0.744
HS2O3-	0.000e+000	0.000e+000	-152.424	-152.593	-0.169
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-134.135	-134.795	-0.660
S(4)	0.000e+000				
SO3-2	0.000e+000	0.000e+000	-45.736	-46.435	-0.700
HSO3-	0.000e+000	0.000e+000	-47.067	-47.236	-0.169
UO2SO3	0.000e+000	0.000e+000	-52.959	-52.959	0.000
H2SO3	0.000e+000	0.000e+000	-53.287	-53.287	0.000
SO2	0.000e+000	0.000e+000	-53.381	-53.381	0.000
UO2(SO3)2-2	0.000e+000	0.000e+000	-97.493	-98.237	-0.744
S2O5-2	0.000e+000	0.000e+000	-98.552	-99.296	-0.744
UO2S2O3	0.000e+000	0.000e+000	-156.680	-156.680	0.000
S3O6-2	0.000e+000	0.000e+000	-175.021	-175.765	-0.744
S4O6-2	0.000e+000	0.000e+000	-266.022	-266.766	-0.744
S5O6-2	0.000e+000	0.000e+000	-385.902	-386.646	-0.744
S(5)	0.000e+000				
S2O6-2	0.000e+000	0.000e+000	-68.114	-68.858	-0.744
S(6)	2.235e-001				
SO4-2	1.350e-001	2.435e-002	-0.870	-1.614	-0.744
NaSO4-	4.949e-002	3.352e-002	-1.306	-1.475	-0.169
TbSO4+	1.463e-002	9.907e-003	-1.835	-2.004	-0.169
Tb(SO4)2-	7.215e-003	4.887e-003	-2.142	-2.311	-0.169
CaSO4	4.424e-003	4.424e-003	-2.354	-2.354	0.000
YbSO4+	1.960e-003	1.328e-003	-2.708	-2.877	-0.169
Yb(SO4)2-	1.439e-003	9.745e-004	-2.842	-3.011	-0.169
MgSO4	5.393e-004	5.393e-004	-3.268	-3.268	0.000
ZnSO4	7.071e-005	7.071e-005	-4.151	-4.151	0.000
KSO4-	5.553e-005	3.761e-005	-4.255	-4.425	-0.169
HSO4-	3.370e-008	2.283e-008	-7.472	-7.642	-0.169
UO2(SO4)2-2	1.873e-012	3.377e-013	-11.727	-12.471	-0.744
UO2SO4	1.565e-012	1.565e-012	-11.805	-11.805	0.000
MnSO4	3.527e-013	3.527e-013	-12.453	-12.453	0.000
KHSO4	3.080e-013	3.080e-013	-12.511	-12.511	0.000
VO2SO4-	2.026e-013	1.372e-013	-12.693	-12.863	-0.169
Al(SO4)2-	1.404e-015	9.508e-016	-14.853	-15.022	-0.169
AlSO4+	7.428e-016	5.031e-016	-15.129	-15.298	-0.169
PuO2SO4	3.719e-016	3.719e-016	-15.430	-15.430	0.000
FeSO4	3.929e-018	3.929e-018	-17.406	-17.406	0.000
FeSO4+	1.266e-018	8.572e-019	-17.898	-18.067	-0.169
Fe(SO4)2-	5.210e-019	3.529e-019	-18.283	-18.452	-0.169
H2SO4	1.999e-019	1.999e-019	-18.699	-18.699	0.000

VOSO4	2.099e-024	2.099e-024	-23.678	-23.678	0.000
Pu(SO4)2-	1.612e-032	1.092e-032	-31.793	-31.962	-0.169
Pu(SO4)2	3.730e-033	3.730e-033	-32.428	-32.428	0.000
PuSO4+	1.062e-033	7.192e-034	-32.974	-33.143	-0.169
PuSO4+2	2.596e-035	5.186e-036	-34.586	-35.285	-0.700
VSO4+	0.000e+000	0.000e+000	-45.493	-45.662	-0.169
U(SO4)2	0.000e+000	0.000e+000	-54.339	-54.339	0.000
USO4+2	0.000e+000	0.000e+000	-55.866	-56.565	-0.700
NH4SO4-	0.000e+000	0.000e+000	-74.546	-74.715	-0.169
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-42.793	-43.537	-0.744
S(8)	2.927e-029				
HSO5-	2.927e-029	1.983e-029	-28.534	-28.703	-0.169
Se(-2)	0.000e+000				
HSe-	0.000e+000	0.000e+000	-95.931	-96.100	-0.169
H2Se	0.000e+000	0.000e+000	-100.311	-100.311	0.000
Se-2	0.000e+000	0.000e+000	-102.270	-103.014	-0.744
Se(4)	1.314e-016				
SeO3-2	1.251e-016	2.256e-017	-15.903	-16.647	-0.744
HSeO3-	6.352e-018	4.302e-018	-17.197	-17.366	-0.169
H2SeO3	1.517e-023	1.517e-023	-22.819	-22.819	0.000
Se(6)	1.916e-004				
SeO4-2	1.915e-004	3.453e-005	-3.718	-4.462	-0.744
ZnSeO4	7.392e-008	7.392e-008	-7.131	-7.131	0.000
HSeO4-	4.024e-011	2.725e-011	-10.395	-10.565	-0.169
MnSeO4	5.456e-016	5.456e-016	-15.263	-15.263	0.000
Si	1.066e-004				
SiO2	9.379e-005	9.379e-005	-4.028	-4.028	0.000
NaHSiO3	1.117e-005	1.117e-005	-4.952	-4.952	0.000
HSiO3-	1.680e-006	1.138e-006	-5.775	-5.944	-0.169
H2SiO4-2	6.433e-011	1.160e-011	-10.192	-10.936	-0.744
H6(H2SiO4)4-2	1.017e-013	1.833e-014	-12.993	-13.737	-0.744
H4(H2SiO4)4-4	1.178e-017	1.066e-020	-16.929	-19.972	-3.043
SiF6-2	0.000e+000	0.000e+000	-95.043	-95.787	-0.744
Tb(2)	0.000e+000				
Tb+2	0.000e+000	0.000e+000	-73.232	-73.932	-0.700
Tb(3)	6.386e-002				
TbCO3+	2.686e-002	1.820e-002	-1.571	-1.740	-0.169
TbSO4+	1.463e-002	9.907e-003	-1.835	-2.004	-0.169
Tb(CO3)2-	9.716e-003	6.580e-003	-2.013	-2.182	-0.169
Tb(SO4)2-	7.215e-003	4.887e-003	-2.142	-2.311	-0.169
Tb+3	2.685e-003	8.243e-005	-2.571	-4.084	-1.513
TbPO4	1.700e-003	1.700e-003	-2.770	-2.770	0.000
TbOH+2	6.496e-004	1.298e-004	-3.187	-3.887	-0.700
Tb(PO4)2-3	2.797e-004	5.556e-006	-3.553	-5.255	-1.702
TbO+	9.052e-005	6.130e-005	-4.043	-4.213	-0.169
TbHPO4+	1.228e-005	8.315e-006	-4.911	-5.080	-0.169
TbHCO3+2	1.097e-005	2.191e-006	-4.960	-5.659	-0.700
TbO2H	8.679e-006	8.679e-006	-5.062	-5.062	0.000
TbNO3+2	1.157e-006	2.312e-007	-5.937	-6.636	-0.700

TbO2-	9.494e-007	6.430e-007	-6.023	-6.192	-0.169
TbCl+2	5.296e-007	1.058e-007	-6.276	-6.976	-0.700
Tb(HPO4)2-	1.559e-008	1.056e-008	-7.807	-7.976	-0.169
TbH2PO4+2	1.628e-009	3.252e-010	-8.788	-9.488	-0.700
TbCl2+	6.037e-011	4.089e-011	-10.219	-10.388	-0.169
TbF+2	9.275e-014	1.852e-014	-13.033	-13.732	-0.700
TbCl3	1.132e-014	1.132e-014	-13.946	-13.946	0.000
TbCl4-	4.334e-018	2.935e-018	-17.363	-17.532	-0.169
TbF2+	4.048e-025	2.742e-025	-24.393	-24.562	-0.169
TbF3	4.612e-037	4.612e-037	-36.336	-36.336	0.000
TbF4-	0.000e+000	0.000e+000	-48.429	-48.598	-0.169
Tc(3)	0.000e+000				
Tc+3	0.000e+000	0.000e+000	-82.011	-83.523	-1.513
Tc(4)	0.000e+000				
TcO(OH)2	0.000e+000	0.000e+000	-47.554	-47.554	0.000
TcOOH+	0.000e+000	0.000e+000	-53.224	-53.394	-0.169
TcO+2	0.000e+000	0.000e+000	-59.585	-60.284	-0.700
(TcO(OH)2)2	0.000e+000	0.000e+000	-88.591	-88.591	0.000
Tc(5)	0.000e+000				
TcO4-3	0.000e+000	0.000e+000	-51.117	-52.819	-1.702
Tc(6)	6.619e-030				
HTcO4-	3.688e-030	2.498e-030	-29.433	-29.602	-0.169
TcO4-2	2.930e-030	5.283e-031	-29.533	-30.277	-0.744
H2TcO4	4.602e-038	4.602e-038	-37.337	-37.337	0.000
Tc(7)	6.088e-008				
TcO4-	6.088e-008	4.123e-008	-7.216	-7.385	-0.169
U(3)	0.000e+000				
U+3	0.000e+000	0.000e+000	-81.895	-83.408	-1.513
U(4)	1.199e-034				
U(OH)4	1.199e-034	1.199e-034	-33.921	-33.921	0.000
U(CO3)4-4	0.000e+000	0.000e+000	-45.777	-48.820	-3.043
U(CO3)5-6	0.000e+000	0.000e+000	-48.651	-55.526	-6.875
UOH+3	0.000e+000	0.000e+000	-52.493	-54.006	-1.513
U(SO4)2	0.000e+000	0.000e+000	-54.339	-54.339	0.000
USO4+2	0.000e+000	0.000e+000	-55.866	-56.565	-0.700
U+4	0.000e+000	0.000e+000	-58.921	-61.486	-2.565
UCl+3	0.000e+000	0.000e+000	-61.407	-62.920	-1.513
UNO3+3	0.000e+000	0.000e+000	-61.610	-63.123	-1.513
U(NO3)2+2	0.000e+000	0.000e+000	-64.700	-65.400	-0.700
UF+3	0.000e+000	0.000e+000	-65.050	-66.563	-1.513
UF2+2	0.000e+000	0.000e+000	-73.275	-73.975	-0.700
UI+3	0.000e+000	0.000e+000	-77.203	-78.716	-1.513
UF3+	0.000e+000	0.000e+000	-82.792	-82.962	-0.169
UF4	0.000e+000	0.000e+000	-93.356	-93.356	0.000
UF5-	0.000e+000	0.000e+000	-106.197	-106.366	-0.169
UF6-2	0.000e+000	0.000e+000	-117.930	-118.674	-0.744
USCN+3	0.000e+000	0.000e+000	-272.031	-273.544	-1.513
U(SCN)2+2	0.000e+000	0.000e+000	-486.579	-487.279	-0.700
U(5)	6.337e-025				
UO2+	6.337e-025	4.292e-025	-24.198	-24.367	-0.169
UO2(CO3)3-5	9.239e-030	1.578e-034	-29.034	-33.802	-4.767

U(6)	3.626e-006				
UO2(CO3)3-4	3.427e-006	3.103e-009	-5.465	-8.508	-3.043
UO2(CO3)2-2	1.606e-007	2.896e-008	-6.794	-7.538	-0.744
UO2(OH)2	2.890e-008	2.890e-008	-7.539	-7.539	0.000
UO2(OH)3-	5.612e-009	3.801e-009	-8.251	-8.420	-0.169
(UO2)2CO3(OH)3-	1.589e-009	1.076e-009	-8.799	-8.968	-0.169
UO2CO3	6.320e-010	6.320e-010	-9.199	-9.199	0.000
UO2PO4-	1.616e-010	1.095e-010	-9.792	-9.961	-0.169
UO2OH+	5.132e-011	3.476e-011	-10.290	-10.459	-0.169
UO2HPO4	2.327e-012	2.327e-012	-11.633	-11.633	0.000
UO2(SO4)2-2	1.873e-012	3.377e-013	-11.727	-12.471	-0.744
UO2SO4	1.565e-012	1.565e-012	-11.805	-11.805	0.000
UO2+2	2.647e-013	5.288e-014	-12.577	-13.277	-0.700
(UO2)3(CO3)6-6	2.592e-013	3.457e-020	-12.586	-19.461	-6.875
UO2(OH)4-2	3.489e-014	6.291e-015	-13.457	-14.201	-0.744
(UO2)3(OH)7-	2.959e-015	2.004e-015	-14.529	-14.698	-0.169
(UO2)3(OH)5+	7.513e-016	5.089e-016	-15.124	-15.293	-0.169
(UO2)2(OH)2+2	3.671e-016	7.332e-017	-15.435	-16.135	-0.700
UO2NO3+	1.219e-016	8.255e-017	-15.914	-16.083	-0.169
UO2Cl+	8.201e-017	5.554e-017	-16.086	-16.255	-0.169
UO2H2PO4+	5.442e-017	3.686e-017	-16.264	-16.433	-0.169
UO2IO3+	2.824e-018	1.913e-018	-17.549	-17.718	-0.169
(UO2)4(OH)7+	1.970e-019	1.334e-019	-18.706	-18.875	-0.169
(UO2)3(OH)4+2	1.109e-019	2.215e-020	-18.955	-19.655	-0.700
(UO2)2OH+3	1.898e-020	5.828e-022	-19.722	-21.235	-1.513
(UO2)3(OH)5CO2+	3.324e-021	2.251e-021	-20.478	-20.648	-0.169
(UO2)3O(OH)2(HCO3)+	2.719e-021	1.842e-021	-20.566	-20.735	-0.169
UO2Cl2	2.008e-021	2.008e-021	-20.697	-20.697	0.000
UO2(H2PO4)2	6.452e-022	6.452e-022	-21.190	-21.190	0.000
UO2F+	4.224e-023	2.861e-023	-22.374	-22.543	-0.169
UO2(IO3)2	2.457e-023	2.457e-023	-22.610	-22.610	0.000
UO2H3PO4+2	7.476e-025	1.493e-025	-24.126	-24.826	-0.700
UO2(H2PO4)(H3PO4)+	9.047e-029	6.127e-029	-28.043	-28.213	-0.169
UO2F2	3.941e-034	3.941e-034	-33.404	-33.404	0.000
UO2ClO3+	3.880e-039	2.628e-039	-38.411	-38.580	-0.169
UO2F3-	0.000e+000	0.000e+000	-45.307	-45.476	-0.169
(UO2)11(CO3)6(OH)12-2	0.000e+000	0.000e+000	-46.342	-47.086	-0.744
UO2SO3	0.000e+000	0.000e+000	-52.959	-52.959	0.000
UO2F4-2	0.000e+000	0.000e+000	-58.295	-59.039	-0.744
UO2(SO3)2-2	0.000e+000	0.000e+000	-97.493	-98.237	-0.744
UO2N3+	0.000e+000	0.000e+000	-110.736	-110.905	-0.169
UO2S2O3	0.000e+000	0.000e+000	-156.680	-156.680	0.000
UO2(N3)2	0.000e+000	0.000e+000	-209.363	-209.363	0.000
UO2SCN+	0.000e+000	0.000e+000	-226.733	-226.902	-0.169
UO2(N3)3-	0.000e+000	0.000e+000	-307.991	-308.161	-0.169
UO2(N3)4-2	0.000e+000	0.000e+000	-408.445	-409.189	-0.744
UO2(SCN)2	0.000e+000	0.000e+000	-442.106	-442.106	0.000
UO2(SCN)3-	0.000e+000	0.000e+000	-656.113	-656.282	-0.169
V(3)	8.392e-038				
V(OH)2+	8.392e-038	5.684e-038	-37.076	-37.245	-0.169

VOH+2	0.000e+000	0.000e+000	-40.913	-41.612	-0.700
VSO4+	0.000e+000	0.000e+000	-45.493	-45.662	-0.169
V+3	0.000e+000	0.000e+000	-45.865	-47.378	-1.513
V2(OH)2+4	0.000e+000	0.000e+000	-79.939	-82.504	-2.565
V(4)	9.923e-023				
VOOH+	9.571e-023	6.482e-023	-22.019	-22.188	-0.169
VOSO4	2.099e-024	2.099e-024	-23.678	-23.678	0.000
VO+2	1.429e-024	2.855e-025	-23.845	-24.544	-0.700
VOF+	1.935e-035	1.310e-035	-34.713	-34.883	-0.169
(VO)2(OH)2+2	9.839e-040	1.965e-040	-39.007	-39.707	-0.700
VOF2	0.000e+000	0.000e+000	-46.441	-46.441	0.000
V(5)	7.451e-003				
VO3OH-2	6.487e-003	1.170e-003	-2.188	-2.932	-0.744
HVO4-2	6.458e-004	1.164e-004	-3.190	-3.934	-0.744
H2VO4-	1.937e-004	1.312e-004	-3.713	-3.882	-0.169
VO2(OH)2-	1.237e-004	8.378e-005	-3.908	-4.077	-0.169
VO4-3	3.487e-008	6.926e-010	-7.458	-9.160	-1.702
VO(OH)3	7.776e-009	7.776e-009	-8.109	-8.109	0.000
VO2+	2.188e-013	1.482e-013	-12.660	-12.829	-0.169
VO2SO4-	2.026e-013	1.372e-013	-12.693	-12.863	-0.169
VO2HPO4-	2.365e-014	1.602e-014	-13.626	-13.795	-0.169
VO2(HPO4)2-3	7.593e-017	1.508e-018	-16.120	-17.822	-1.702
VO2F	1.523e-024	1.523e-024	-23.817	-23.817	0.000
VO2H2PO4	1.053e-026	1.053e-026	-25.978	-25.978	0.000
VO2F2-	2.977e-036	2.016e-036	-35.526	-35.696	-0.169
Yb(2)	1.960e-035				
Yb+2	1.960e-035	3.914e-036	-34.708	-35.407	-0.700
Yb(3)	2.001e-002				
YbCO3+	9.874e-003	6.688e-003	-2.005	-2.175	-0.169
Yb(CO3)2-	4.867e-003	3.296e-003	-2.313	-2.482	-0.169
YbSO4+	1.960e-003	1.328e-003	-2.708	-2.877	-0.169
Yb(SO4)2-	1.439e-003	9.745e-004	-2.842	-3.011	-0.169
YbPO4	8.515e-004	8.515e-004	-3.070	-3.070	0.000
Yb+3	4.253e-004	1.306e-005	-3.371	-4.884	-1.513
Yb(PO4)2-3	3.519e-004	6.990e-006	-3.454	-5.156	-1.702
YbOH+2	1.706e-004	3.408e-005	-3.768	-4.468	-0.700
YbO+	3.912e-005	2.650e-005	-4.408	-4.577	-0.169
YbO2H	2.083e-005	2.083e-005	-4.681	-4.681	0.000
YbO2-	5.189e-006	3.514e-006	-5.285	-5.454	-0.169
YbHPO4+	3.082e-006	2.087e-006	-5.511	-5.680	-0.169
YbHCO3+2	2.413e-006	4.819e-007	-5.618	-6.317	-0.700
YbNO3+2	9.307e-008	1.859e-008	-7.031	-7.731	-0.700
YbCl+2	7.096e-008	1.417e-008	-7.149	-7.849	-0.700
Yb(HPO4)2-	7.809e-009	5.289e-009	-8.107	-8.277	-0.169
YbH2PO4+2	3.591e-010	7.172e-011	-9.445	-10.144	-0.700
YbCl2+	5.854e-012	3.965e-012	-11.233	-11.402	-0.169
YbF+2	2.065e-014	4.124e-015	-13.685	-14.385	-0.700
YbCl3	8.967e-016	8.967e-016	-15.047	-15.047	0.000
YbCl4-	3.463e-019	2.345e-019	-18.461	-18.630	-0.169
YbF2+	1.073e-025	7.270e-026	-24.969	-25.138	-0.169
YbF3	1.657e-037	1.657e-037	-36.781	-36.781	0.000

YbF4-	0.000e+000	0.000e+000	-48.777	-48.946	-0.169
Zn	1.286e-004				
ZnSO4	7.071e-005	7.071e-005	-4.151	-4.151	0.000
Zn+2	5.408e-005	1.382e-005	-4.267	-4.859	-0.593
ZnOH+	2.377e-006	1.610e-006	-5.624	-5.793	-0.169
Zn(OH)2	7.322e-007	7.322e-007	-6.135	-6.135	0.000
ZnCO3	2.765e-007	2.765e-007	-6.558	-6.558	0.000
ZnHCO3+	2.621e-007	1.775e-007	-6.582	-6.751	-0.169
ZnSeO4	7.392e-008	7.392e-008	-7.131	-7.131	0.000
Zn(OH)Cl	2.977e-008	2.977e-008	-7.526	-7.526	0.000
ZnCl+	2.421e-008	1.640e-008	-7.616	-7.785	-0.169
ZnPO4-	1.755e-008	1.188e-008	-7.756	-7.925	-0.169
ZnHPO4	4.021e-009	4.021e-009	-8.396	-8.396	0.000
Zn(OH)3-	3.558e-010	2.410e-010	-9.449	-9.618	-0.169
ZnCl2	1.352e-011	1.352e-011	-10.869	-10.869	0.000
Zn(OH)4-2	2.420e-014	4.364e-015	-13.616	-14.360	-0.744
ZnCl3-	7.785e-015	5.273e-015	-14.109	-14.278	-0.169
ZnCl4-2	1.565e-016	2.822e-017	-15.805	-16.549	-0.744
ZnF+	1.323e-018	8.961e-019	-17.878	-18.048	-0.169
ZnH2PO4+	8.149e-020	5.519e-020	-19.089	-19.258	-0.169
ZnI+	7.103e-027	4.811e-027	-26.149	-26.318	-0.169
ZnClO4+	3.356e-030	2.273e-030	-29.474	-29.643	-0.169
ZnI2	0.000e+000	0.000e+000	-43.593	-43.593	0.000
ZnI3-	0.000e+000	0.000e+000	-62.030	-62.200	-0.169
Zn(NH3)+2	0.000e+000	0.000e+000	-68.116	-68.816	-0.700
ZnI4-2	0.000e+000	0.000e+000	-80.500	-81.244	-0.744
ZnN3+	0.000e+000	0.000e+000	-104.456	-104.625	-0.169
Zn(NH3)2+2	0.000e+000	0.000e+000	-131.919	-132.619	-0.700
Zn(NH3)3+2	0.000e+000	0.000e+000	-195.722	-196.421	-0.700
Zn(N3)2	0.000e+000	0.000e+000	-204.080	-204.080	0.000
Zn(NH3)4+2	0.000e+000	0.000e+000	-259.798	-260.498	-0.700
Zn(SCN)2	0.000e+000	0.000e+000	-434.051	-434.051	0.000
Zn(CN)4-2	0.000e+000	0.000e+000	-481.542	-482.286	-0.744
Zn(SCN)4-2	0.000e+000	0.000e+000	-863.012	-863.756	-0.744

Saturation indices

Phase	SI	log IAP	log KT	
(UO2)2As2O7	-77.27	-69.59	7.68	(UO2)2As2O7
(UO2)2Cl3	-59.78	-48.58	11.20	(UO2)2Cl3
(UO2)2P2O7	-25.37	-40.14	-14.77	(UO2)2P2O7
(UO2)3(AsO4)2	-76.10	-66.80	9.29	(UO2)3(AsO4)2
(UO2)3(PO4)2	-23.26	-37.36	-14.10	(UO2)3(PO4)2
(UO2)3(PO4)2:4H2O	-10.33	-37.38	-27.05	(UO2)3(PO4)2:4H2O
(VO)3(PO4)2	-119.95	-121.90	-1.96	(VO)3(PO4)2
Afwillite	-28.58	31.39	59.96	Ca3Si2O4(OH)6
Akermanite	-15.00	30.23	45.23	Ca2MgSi2O7
Al	-139.83	-54.41	85.42	Al
Al(g)	-190.53	-54.41	136.12	Al
Al2(SO4)3	-57.13	-38.23	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-39.82	-38.27	1.56	Al2(SO4)3:6H2O

Alabandite	-145.52	-179.65	-34.13	MnS
Albite	-0.00	2.66	2.66	NaAlSi3O8
Albite_high	-1.32	2.66	3.98	NaAlSi3O8
Albite_low	-0.00	2.66	2.66	NaAlSi3O8
AlF3	-42.44	-59.71	-17.27	AlF3
Alstonite	-4.43	-1.84	2.58	BaCa(CO3)2
Alum-K	-18.74	-23.72	-4.97	KAl(SO4)2:12H2O
Alunite	-8.40	-8.87	-0.47	KAl3(OH)6(SO4)2
Amesite-14A	-5.87	69.40	75.27	Mg4Al4Si2O10(OH)8
Analcime	-0.13	5.93	6.06	Na.96Al.96Si2.04O6:H2O
Analcime-dehy	-6.49	5.93	12.42	Na.96Al.96Si2.04O6
Andalusite	-5.12	10.76	15.88	Al2SiO5
Andradite	5.49	64.71	59.22	Ca3Fe2(SiO4)3
Anhydrite	-0.17	-4.52	-4.35	CaSO4
Annite	-35.52	-6.19	29.33	KFe3AlSi3O10(OH)2
Anorthite	-6.59	19.88	26.48	CaAl2(SiO4)2
Antarcticite	-13.34	-9.25	4.09	CaCl2:6H2O
Anthophyllite	-14.87	51.61	66.48	Mg7Si8O22(OH)2
Antigorite	-37.86	437.77	475.63	Mg48Si34O85(OH)62
Aphthitalite	-11.17	-15.06	-3.89	NaK3(SO4)2
Aragonite	-0.15	1.82	1.97	CaCO3
Arcanite	-7.21	-9.05	-1.84	K2SO4
Arsenolite	-112.78	-157.55	-44.77	As2O3
Arsenopyrite	-262.21	-324.99	-62.78	FeAsS
Artinite	-7.03	12.60	19.63	Mg2CO3(OH)2:3H2O
As	-106.30	-140.58	-34.28	As
As2O5	-77.28	-75.15	2.14	As2O5
As4O6(cubi)	-225.42	-315.10	-89.69	As4O6
As4O6(mono)	-225.19	-315.10	-89.91	As4O6
Autunite-H	-14.79	-40.15	-25.35	H2(UO2)2(PO4)2
B	-107.51	-62.45	45.06	B
B(g)	-198.80	-62.45	136.35	B
B2O3	-6.84	-1.30	5.55	B2O3
Ba	-131.77	-33.54	98.23	Ba
Ba(OH)2:8H2O	-16.89	7.60	24.49	Ba(OH)2:8H2O
Ba2Si3O8	-19.99	3.24	23.23	Ba2Si3O8
Ba2SiO4	-33.26	11.29	44.55	Ba2SiO4
Ba2U2O7	-53.81	-20.32	33.49	Ba2U2O7
Ba3UO6	-68.60	25.76	94.36	Ba3UO6
BaCl2	-16.93	-14.70	2.23	BaCl2
BaCl2:2H2O	-14.92	-14.71	0.21	BaCl2:2H2O
BaCl2:H2O	-15.53	-14.71	0.82	BaCl2:H2O
BaHPO4	-7.79	-15.19	-7.40	BaHPO4
BaI2	-56.33	-267.94	-211.61	BaI2
BaMnO4	-15.47	92.89	108.36	BaMnO4
BaO	-40.14	7.66	47.80	BaO
Barite	0.00	-10.01	-10.01	BaSO4
Barytocalcite	-4.59	-1.84	2.74	BaCa(CO3)2
BaS	-157.35	-174.82	-17.47	BaS
BaSeO3	-18.47	-54.06	-35.59	BaSeO3
BaSeO4	-5.40	-12.86	-7.46	BaSeO4

BaSiF6	-98.36	-130.57	-32.22	BaSiF6
Bassanite	-0.82	-4.52	-3.71	CaSO4:0.5H2O
Bassetite	-24.33	-42.07	-17.74	Fe(UO2)2(PO4)2
BaU2O7	-8.74	13.22	21.96	BaU2O7
BaUO4	-7.75	10.44	18.19	BaUO4
Beidellite-Ca	-0.84	4.61	5.44	Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H	-2.05	2.44	4.49	H.33Al2.33Si3.67O10(OH)2
Beidellite-K	-1.30	3.86	5.16	K.33Al2.33Si3.67O10(OH)2
Beidellite-Mg	-0.99	4.41	5.41	Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na	-0.64	4.86	5.50	Na.33Al2.33Si3.67O10(OH)2
Berlinite	-8.19	-15.46	-7.27	AlPO4
BF3(g)	-64.77	-67.75	-2.98	BF3
Birnessite	0.00	269.79	269.79	Mn8O14:5H2O
Bischofite	-14.81	-10.42	4.39	MgCl2:6H2O
Bixbyite	-3.33	46.86	50.18	Mn2O3
Bloedite	-6.22	-8.70	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-0.16	7.39	7.55	AlO2H
Boltwoodite	-11.83	3.06	14.89	K(H3O)(UO2)SiO4
Boltwoodite-Na	-9.41	5.18	14.58	Na.7K.3(H3O)(UO2)SiO4:H2O
Borax	0.00	12.04	12.04	Na2(B4O5(OH)4):8H2O
Boric_acid	-0.50	-0.66	-0.16	B(OH)3
Brucite	-4.31	11.97	16.28	Mg(OH)2
Brushite	-16.26	-9.71	6.55	CaHPO4:2H2O
Burkeite	-12.07	-2.58	9.49	Na6CO3(SO4)2
C	-71.88	-93.73	-21.85	C
C(g)	-189.50	-93.73	95.77	C
Ca	-124.88	-28.05	96.83	Ca
Ca(g)	-150.12	-28.05	122.07	Ca
Ca-Al_Pyroxene	-11.99	23.91	35.90	CaAl2SiO6
Ca2Al2O5:8H2O	-18.53	41.04	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-22.36	3.93	26.29	Ca2Cl2(OH)2:H2O
Ca2V2O7	-0.48	16.71	17.18	Ca2V2O7
Ca3(AsO4)2	-53.49	-35.69	17.80	Ca3(AsO4)2
Ca3Al2O6	-58.79	54.25	113.03	Ca3Al2O6
Ca3V2O8	-8.71	29.86	38.57	Ca3V2O8
Ca4Al2Fe2O10	-61.79	104.73	166.52	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-39.94	67.32	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-36.40	67.28	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-38.18	30.15	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-18.97	27.94	46.91	CaAl2O4
CaAl2O4:10H2O	-10.12	27.88	37.99	CaAl2O4:10H2O
CaAl4O7	-25.87	42.73	68.59	CaAl4O7
Calcite	-0.00	1.82	1.82	CaCO3
Carnallite	-21.56	-17.29	4.27	KMgCl3:6H2O
Carnotite	4.07	4.59	0.51	K2(UO2)2(VO4)2
CaSeO3:2H2O	-14.93	-48.58	-33.65	CaSeO3:2H2O
CaSeO4	-4.28	-7.37	-3.09	CaSeO4

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      CaSO4:0.5H2O(beta)  -0.99   -4.52   -3.54  CaSO4:0.5H2O
      CaUO4            -0.00   15.94   15.94  CaUO4
      CaV2O6           -1.98    3.55    5.53  CaV2O6
      Celadonite        0.25    7.56    7.31  KMgAlSi4O10(OH)2
      CH4(g)         -145.41 -176.15  -30.74  CH4
      Chalcedony       -0.27   -4.03   -3.76  SiO2

      Chamosite-7A    -25.88    6.88   32.76  Fe2Al2SiO5(OH)4
      Chloromagnesite -32.20  -10.38   21.82  MgCl2
      Chrysotile       -3.17   27.86   31.03  Mg3Si2O5(OH)4
      Cl2(g)          -27.15   18.84   45.99  Cl2
      Claudetite     -112.83 -157.55  -44.73  As2O3
      Clinochlore-14A  -4.49   62.56   67.05  Mg5Al2Si3O10(OH)8
      Clinochlore-7A   -7.86   62.56   70.42  Mg5Al2Si3O10(OH)8
      Clinoptilolite-Ca  -2.69   -9.98   -7.29
Ca1.7335Al3.45Fe.017Si14.533O36:10.922H2O
      Clinoptilolite-dehy-Ca -38.27   -9.91   28.36
Ca1.7335Al3.45Fe.017Si14.533O36
      Clinoptilolite-dehy-K -42.19  -17.77   24.43
K3.467Al3.45Fe.017Si14.533O36
      Clinoptilolite-dehy-Na -35.47   -7.24   28.23
Na3.467Al3.45Fe.017Si14.533O36
      Clinoptilolite-dehy-NH4-254.96 -642.68 -387.72
(NH4)3.467Al3.45Fe.017Si14.533O36
      Clinoptilolite-hy-Ca  -2.69   -9.99   -7.29
Ca1.7335Al3.45Fe.017Si14.533O36:11.645H2O
      Clinoptilolite-hy-K  -6.58  -17.81  -11.23
K3.467Al3.45Fe.017Si14.533O36:7.499H2O
      Clinoptilolite-hy-Na   0.12   -7.31   -7.43
Na3.467Al3.45Fe.017Si14.533O36:10.877H2O
      Clinoptilolite-K  -6.61  -17.84  -11.23
K3.467Al3.45Fe.017Si14.533O36:10.922H2O
      Clinoptilolite-Na   0.12   -7.31   -7.42
Na3.467Al3.45Fe.017Si14.533O36:10.922H2O
      Clinoptilolite-NH4-219.39 -642.75 -423.36
(NH4)3.467Al3.45Fe.017Si14.533O36:10.922H2O
      Clinozoisite     -6.70   36.40   43.10  Ca2Al3Si3O12(OH)
      CO(g)           -48.21  -52.53   -4.32  CO
      CO2(g)           -3.50  -11.33   -7.83  CO2
      Coesite          -0.81   -4.03   -3.22  SiO2
      Coffinite       -25.33  -42.45  -17.12  USiO4
      Colemanite        0.87   22.39   21.51  Ca2B6O11:5H2O
      Cordierite_anhyd -18.68   33.39   52.07  Mg2Al4Si5O18
      Cordierite_hydr -16.20   33.38   49.59  Mg2Al4Si5O18:H2O
      Corundum         -3.50   14.79   18.29  Al2O3
      Cristobalite(alpha)  -0.55   -4.03   -3.48  SiO2
      Cristobalite(beta)  -0.99   -4.03   -3.03  SiO2
      Cronstedtite-7A -12.79   29.43   42.21  Fe2Fe2SiO5(OH)4
      Daphnite-14A    -59.09   -6.99   52.10  Fe5AlAlSi3O10(OH)8
      Daphnite-7A     -62.47   -6.99   55.48  Fe5AlAlSi3O10(OH)8
      Dawsonite        -0.93    3.41    4.34  NaAlCO3(OH)2
      Diaspore          0.24    7.39    7.15  AlHO2
      Dicalcium_silicate -14.85   22.28   37.13  Ca2SiO4
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      Diopside          -3.81   17.07   20.89  CaMgSi2O6
      Dolomite          -0.00    2.47    2.47  CaMg(CO3)2
      Dolomite-dis      -1.54    2.47    4.01  CaMg(CO3)2
      Dolomite-ord       0.01    2.47    2.46  CaMg(CO3)2
      Downeyite        -25.92  -61.72  -35.81  SeO2
      Enstatite         -3.34    7.95   11.29  MgSiO3

      Epidote            1.88   47.67   45.79  Ca2FeAl2Si3O12OH
      Epidote-ord        1.89   47.67   45.78  FeCa2Al2(OH)(SiO4)3
      Epsomite          -3.78   -5.74   -1.96  MgSO4:7H2O
      Ettringite       -21.98   40.49   62.46
Ca6Al2(SO4)3(OH)12:26H2O
      F2(g)           -102.24   -3.53   98.71  F2
      Fayalite         -26.96   -7.90   19.06  Fe2SiO4
      Fe               -59.15  -43.13   16.02  Fe
      Fe(OH)2          -15.83   -1.94   13.89  Fe(OH)2
      Fe(OH)3            0.00   18.66   18.66  Fe(OH)3
      Fe2(SO4)3        -44.77  -15.68   29.08  Fe2(SO4)3
      FeF2             -44.24  -46.67   -2.42  FeF2
      FeF3             -42.20  -48.44   -6.24  FeF3
      FeO              -15.46   -1.93   13.52  FeO
      Ferrite-Ca         2.96   50.49   47.53  CaFe2O4
      Ferrite-Dicalcium -19.19   63.64   82.84  Ca2Fe2O5
      Ferrite-Mg         2.25   49.31   47.06  MgFe2O4
      Ferrite-Zn        10.80   48.53   37.74  ZnFe2O4
      Ferroselite     -152.57 -331.38 -178.81  FeSe2
      Ferrosilite      -13.37   -5.96    7.41  FeSiO3
      FeSO4            -22.21  -19.61    2.61  FeSO4
      FeV2O4          -329.07  -93.94  235.14  FeV2O4
      Fluorapatite       0.00  -25.16  -25.16  Ca5(PO4)3F
      Fluorite         -21.51  -31.58  -10.07  CaF2
      Forsterite        -7.88   19.93   27.81  Mg2SiO4
      Foshagite        -25.28   40.52   65.80  Ca4Si3O9(OH)2:0.5H2O
      Frankdicksonite  -31.32  -37.08   -5.76  BaF2
      Gaylussite        -6.00    5.16   11.16  CaNa2(CO3)2:5H2O
      Gehlenite        -19.16   37.06   56.22  Ca2Al2SiO7
      Gibbsite          -0.36    7.38    7.74  Al(OH)3
      Gismondine        -2.01   39.71   41.72  Ca2Al4Si4O16:9H2O
      Glauberite        -2.03   -7.49   -5.47  Na2Ca(SO4)2
      Goethite           5.12   18.66   13.55  FeOOH
      Greenalite       -36.45  -13.87   22.58  Fe3Si2O5(OH)4
      Grossular         -9.61   42.16   51.78  Ca3Al2(SiO4)3
      Gypsum            -0.00   -4.53   -4.53  CaSO4:2H2O
      Gyrolite          -8.60   14.21   22.80  Ca2Si3O7(OH)2:1.5H2O
      H2(g)            -41.21  -41.21   -0.00  H2
      H2O(g)            -1.59   -0.01    1.59  H2O
      H2S(g)          -140.78 -182.48  -41.70  H2S
      Haiweeite          1.56   -5.48   -7.04  Ca(UO2)2(Si2O5)3:5H2O
      Halite            -5.40   -3.83    1.56  NaCl
      Hatrurite        -37.92   35.43   73.35  Ca3SiO5
      Hausmannite      -11.61   49.68   61.29  Mn3O4
      HCl(g)           -17.49  -11.18    6.30  HCl
      Hedenbergite     -16.36    3.16   19.53  CaFe(SiO3)2
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Hematite	11.22	37.33	26.11	Fe2O3
Hercynite	-15.95	12.85	28.80	FeAl2O4
Hexahydrite	-4.01	-5.73	-1.73	MgSO4:6H2O
HI(g)	-35.87	-137.80	-101.93	HI
Hillebrandite	-14.50	22.27	36.77	Ca2SiO3(OH)2:0.17H2O
Hopeite	-1.47	-12.13	-10.66	Zn3(PO4)2:4H2O
HTcO4	-21.37	-15.42	5.95	HTcO4
Huntite	-6.45	3.77	10.22	CaMg3(CO3)4
Hydroboracite	0.84	21.20	20.36	MgCaB6O11:6H2O
Hydromagnesite	-16.20	14.54	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.95	-9.21	11.75	CaCl2
Hydroxylapatite	0.43	-2.79	-3.22	Ca5(OH)(PO4)3
Hydrozincite	3.01	33.32	30.31	Zn5(OH)6(CO3)2
I2	-29.91	-234.40	-204.49	I2
I2(g)	-33.32	-234.40	-201.08	I2
Ice	-0.15	-0.01	0.14	H2O
Illite	-0.40	8.48	8.88	
K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2				
Jadeite	-1.62	6.69	8.31	NaAl(SiO3)2
Jarosite	-4.70	24.95	29.64	KFe3(SO4)2(OH)6
Jarosite-Na	-5.62	27.99	33.61	NaFe3(SO4)2(OH)6
K	-65.77	-16.29	49.48	K
K(g)	-76.37	-16.29	60.08	K
K-Feldspar	-0.00	-0.38	-0.38	KAlSi3O8
K2CO3:1.5H2O	-16.09	-2.72	13.38	K2CO3:1.5H2O
K2O	-75.41	8.62	84.04	K2O
K2Se	-121.74	-176.70	-54.97	K2Se
K2UO4	-22.47	11.40	33.87	K2UO4
K3H(SO4)2	-18.79	-22.41	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-61.22	-33.51	27.71	K8H4(CO3)6:3H2O
Kainite	-12.27	-12.58	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-26.91	-23.64	3.27	KAl(SO4)2
Kalicinite	-7.30	-7.02	0.28	KHCO3
Kalsilite	-3.17	7.68	10.85	KAlSiO4
Kaolinite	0.00	6.72	6.72	Al2Si2O5(OH)4
Karelianite	-56.53	-92.00	-35.47	V2O3
Katoite	-24.74	54.21	78.94	Ca3Al2H12O12
Kieserite	-5.43	-5.70	-0.27	MgSO4:H2O
KMgCl3	-38.50	-17.25	21.25	KMgCl3
KMgCl3:2H2O	-31.23	-17.27	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-9.97	0.29	10.26	KNaCO3:6H2O
KTcO4	-8.83	-11.10	-2.27	KTcO4
KUO2AsO4	-26.31	-30.48	-4.17	KUO2AsO4
Kyanite	-4.85	10.76	15.61	Al2SiO5
Lansfordite	-4.22	0.62	4.84	MgCO3:5H2O
Larnite	-16.14	22.28	38.42	Ca2SiO4
Laumontite	-1.71	11.80	13.51	CaAl2Si4O12:4H2O
Lawrencite	-33.35	-24.29	9.05	FeCl2
Lawsonite	-2.23	19.87	22.11	CaAl2Si2O7(OH)2:H2O
Leonite	-10.66	-14.77	-4.11	K2Mg(SO4)2:4H2O
Lime	-19.42	13.15	32.57	CaO
Magnesite	-1.62	0.65	2.27	MgCO3

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      Magnetite          -1.05   35.40   36.45  Fe3O4
      Manganite          -1.98   23.42   25.41  MnO(OH)
      Manganosite       -15.09    2.83   17.92  MnO
      Margarite          -6.26   34.66   40.93  CaAl4Si2O10(OH)2
      Maximum_Microcline   0.00   -0.38   -0.38  KAlSi3O8
      Mayenite          -232.81  261.34  494.15  Ca12Al14O33

      Melanterite       -17.25  -19.65   -2.40  FeSO4:7H2O
      Mercallite        -11.93  -13.36   -1.44  KHSO4
      Merwinite         -25.03   43.38   68.41  MgCa3(SiO4)2
      Mesolite            2.69   16.18   13.49
Na.676Ca.657Al1.99Si3.01O10:2.647H2O
      Mg                -108.75  -29.22   79.52  Mg
      Mg(g)             -128.47  -29.22   99.25  Mg
      Mg1.25SO4(OH)0.5:0.5H2O  -7.90   -2.71    5.20
Mg1.25SO4(OH)0.5:0.5H2O
      Mg1.5SO4(OH)       -8.92    0.29    9.21  Mg1.5SO4(OH)
      Mg2V2O7           -11.64   14.36   25.99  Mg2V2O7
      MgCl2:2H2O        -23.13  -10.40   12.73  MgCl2:2H2O
      MgCl2:4H2O        -17.71  -10.41    7.30  MgCl2:4H2O
      MgCl2:H2O         -26.46  -10.39   16.07  MgCl2:H2O
      MgOHCl            -15.10    0.79   15.89  MgOHCl
      MgSeO3            -22.40  -49.74  -27.34  MgSeO3
      MgSeO3:6H2O       -17.33  -49.78  -32.45  MgSeO3:6H2O
      MgSO4             -10.52   -5.69    4.83  MgSO4
      MgUO4              -8.23   14.76   22.99  MgUO4
      MgV2O6             -8.67    2.38   11.05  MgV2O6
      Minnesotaite      -35.75  -21.92   13.83  Fe3Si4O10(OH)2
      Mirabilite         -1.88   -3.04   -1.15  Na2SO4:10H2O
      Misenite          -78.16  -89.23  -11.08  K8H6(SO4)7
      Mn                -78.31  -38.37   39.94  Mn
      Mn(OH)2(am)       -12.49    2.82   15.31  Mn(OH)2
      Mn(OH)3            -8.50   23.42   31.92  Mn(OH)3
      Mn3(PO4)2         -38.04  -37.22    0.82  Mn3(PO4)2
      MnCl2:2H2O        -23.54  -19.55    4.00  MnCl2:2H2O
      MnCl2:4H2O        -22.31  -19.56    2.75  MnCl2:4H2O
      MnCl2:H2O         -25.08  -19.54    5.54  MnCl2:H2O
      MnHPO4             -7.08  -20.03  -12.95  MnHPO4
      MnO2(gamma)         0.93   44.03   43.10  MnO2
      MnSe              -105.55 -182.50  -76.95  MnSe
      MnSeO3            -22.61  -58.89  -36.29  MnSeO3
      MnSeO3:2H2O       -23.56  -58.91  -35.35  MnSeO3:2H2O
      MnSO4             -17.45  -14.84    2.61  MnSO4
      MnV2O6            -11.59   -6.77    4.82  MnV2O6
      Molysite          -41.36  -14.87   26.49  FeCl3
      Monohydrocalcite   -0.86    1.82    2.68  CaCO3:H2O
      Monticellite       -8.43   21.10   29.53  CaMgSiO4
      Montmor-Ca          0.01    2.35    2.34
Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K          -0.39    1.60    1.99  K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg         -0.08    2.16    2.23  Mg.495Al1.67Si4O10(OH)2
Montmor-Na          0.28    2.61    2.33  Na.33Mg.33Al1.67Si4O10(OH)2
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Mordenite	-1.63	-6.99	-5.36	Ca.2895Na.361Al.94Si5.06O12:3.468H2O
Mordenite-dehy	-16.74	-6.97	9.77	Ca.2895Na.361Al.94Si5.06O12
Muscovite	0.95	14.40	13.45	KAl3Si3O10(OH)2
N2(g)	-17.75	-228.24	-210.49	N2
Na	-59.12	-13.25	45.87	Na
Na(g)	-72.61	-13.25	59.36	Na
Na2CO3	-7.80	3.37	11.16	Na2CO3
Na2CO3:7H2O	-6.62	3.32	9.94	Na2CO3:7H2O
Na2O	-52.72	14.70	67.42	Na2O
Na2Se	-116.21	-170.63	-54.42	Na2Se
Na2Se2	-163.89	-314.75	-150.86	Na2Se2
Na2SiO3	-11.53	10.67	22.20	Na2SiO3
Na2U2O7	-2.33	20.26	22.59	Na2U2O7
Na2UO4(alpha)	-12.54	17.48	30.02	Na2UO4
Na3H(SO4)2	-12.41	-13.30	-0.89	Na3H(SO4)2
Na3UO4	-50.53	4.23	54.76	Na3UO4
Na4Ca(SO4)3:2H2O	-4.59	-10.48	-5.89	Na4Ca(SO4)3:2H2O
Na4SiO4	-45.23	25.36	70.60	Na4SiO4
Na4UO2(CO3)3	-5.85	-1.81	4.04	Na4UO2(CO3)3
Na6Si2O7	-65.50	36.03	101.53	Na6Si2O7
NaFeO2	-6.89	26.02	32.90	NaFeO2
Nahcolite	-3.84	-3.98	-0.14	NaHCO3
NaTcO4	-9.59	-8.07	1.52	NaTcO4
Natrolite	-1.00	17.39	18.39	Na2Al2Si3O10:2H2O
Natron	-6.28	3.30	9.59	Na2CO3:10H2O
Natrosilite	-11.42	6.64	18.07	Na2Si2O5
NaUO3	-17.32	-10.47	6.85	NaUO3
Nepheline	-3.04	10.71	13.75	NaAlSiO4
Nesquehonite	-4.66	0.63	5.29	MgCO3:3H2O
NH3(g)	-67.81	-175.93	-108.13	NH3
NH4HSe	-163.03	-361.26	-198.23	NH4HSe
Ningyoite	-32.12	-70.98	-38.86	CaUP2O8:2H2O
Niter	-6.58	-6.81	-0.22	KNO3
Nitrobarite	-12.08	-14.57	-2.49	Ba(NO3)2
NO(g)	-24.39	-72.92	-48.53	NO
NO2(g)	-18.57	-31.72	-13.15	NO2
Nontronite-Ca	12.85	27.16	14.31	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	11.64	24.98	13.35	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	12.38	26.41	14.02	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	12.69	26.96	14.27	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	13.05	27.41	14.36	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-0.70	82.40	83.10	O2
Okenite	-5.23	5.09	10.31	CaSi2O4(OH)2:H2O
Orpiment	-499.45	-704.98	-205.54	As2S3
Oxychloride-Mg	-13.09	12.74	25.83	Mg2Cl(OH)3:4H2O
P	-150.41	-125.86	24.56	P

Paragonite	0.06	17.44	17.38	NaAl3Si3O10(OH)2
Pargasite	-22.13	79.57	101.70	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrite	-4.34	-5.73	-1.39	MgSO4:5H2O
Periclase	-9.35	11.98	21.33	MgO
Phlogopite	-1.75	35.55	37.30	KAlMg3Si3O10(OH)2
Picromerite	-10.34	-14.78	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-6.14	5.18	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-9.48	-23.79	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-9.40	13.15	22.55	Ca(OH)2
Prehnite	-3.79	29.00	32.79	Ca2Al2Si3O10(OH)2
Pseudowollastonite	-4.84	9.13	13.96	CaSiO3
Pu	-174.14	-108.33	65.81	Pu
Pu(HPO4)2	-25.31	-71.64	-46.33	Pu(HPO4)2
Pu(OH)3	-33.43	-46.54	-13.11	Pu(OH)3
Pu(OH)4	-8.14	-25.94	-17.81	Pu(OH)4
Pu2O3	-70.07	-93.06	-22.98	Pu2O3
PuF3	-67.83	-113.63	-45.80	PuF3
PuF4	-83.55	-115.40	-31.85	PuF4
PuO2	0.00	-25.93	-25.93	PuO2
PuO2(OH)2	-4.59	15.27	19.86	PuO2(OH)2
PuO2HPO4	-11.24	-7.58	3.66	PuO2HPO4
PuO2OH(am)	-10.79	-5.33	5.46	PuO2OH
Pyrite	-242.00	-325.69	-83.69	FeS2
Pyrolusite	2.47	44.03	41.56	MnO2
Pyrophyllite	-1.62	-1.33	0.29	Al2Si4O10(OH)2
Pyrrhotite	-146.96	-184.41	-37.45	FeS
Quartz	0.00	-4.03	-4.03	SiO2
Rankinite	-20.42	31.40	51.82	Ca3Si2O7
Realgar	-200.74	-281.85	-81.11	AsS
Rhodochrosite	-8.28	-8.50	-0.22	MnCO3
Rhodonite	-10.89	-1.20	9.69	MnSiO3
Ripidolite-14A	-26.04	34.74	60.78	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	-29.42	34.74	64.16	Mg3Fe2Al2Si3O10(OH)8
Rutherfordine	-4.43	-8.55	-4.12	UO2CO3
S	-105.46	-141.28	-35.82	S
S2(g)	-224.80	-282.55	-57.75	S2
Saleeite	-8.69	-28.16	-19.48	Mg(UO2)2(PO4)2
Sanbornite	-9.80	-0.40	9.41	BaSi2O5
Sanidine_high	-1.20	-0.38	0.82	KAlSi3O8
Saponite-Ca	-0.39	25.75	26.14	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	-1.60	23.58	25.18	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	-0.85	25.01	25.86	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	-0.54	25.56	26.10	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	-0.19	26.01	26.20	Na.33Mg3Al.33Si3.67O10(OH)2
Scacchite	-28.27	-19.53	8.74	MnCl2
Schoepite	-2.07	2.77	4.83	UO3:2H2O
Schoepite-dehy(.393)	-3.95	2.78	6.72	UO3:.393H2O

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      Schoepite-dehy(.648)  -3.43    2.78    6.21  UO3:.648H2O
      Schoepite-dehy(.85)  -2.32    2.78    5.10  UO3:.85H2O
      Schoepite-dehy(.9)  -2.24    2.78    5.02  UO3:.9H2O

      Schoepite-dehy(1.0)  -2.33    2.78    5.10  UO3:H2O
      Scolecite          0.09   15.84   15.75  CaAl2Si3O10:3H2O
      Se               -55.21 -144.12  -88.92  Se
      Se2O5            -62.72  -82.24  -19.53  Se2O5
      SeCl4            -91.76 -106.44  -14.68  SeCl4
      Sellaite         -23.31  -32.76   -9.44  MgF2
      SeO3             -39.68  -20.52   19.16  SeO3
      Sepiolite         -6.52   23.70   30.22  Mg4Si6O15(OH)2:6H2O
      Shcherbinaite     -8.15   -9.60   -1.45  V2O5
      Si               -149.30  -86.43   62.87  Si
      Si(g)            -220.37  -86.43  133.94  Si
      Siderite         -13.04  -13.26   -0.22  FeCO3
      SiF4(g)          -78.26  -93.50  -15.24  SiF4
      Sillimanite       -5.49   10.76   16.24  Al2SiO5
      SiO2(am)          -1.29   -4.03   -2.74  SiO2
      Sklodowskite      -4.35    9.44   13.79
Mg(H3O)2(UO2)2(SiO4)2:4H2O
      Smectite-high-Fe-Mg  -6.27   13.60   19.88
Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
      Smectite-low-Fe-Mg  -3.41    9.56   12.98
Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
      Smithsonite       -0.57   -0.13    0.44  ZnCO3
      SO2(g)           -53.56  -58.87   -5.32  SO2
      Soddyite           1.13    1.52    0.39  (UO2)2SiO4:2H2O
      Sphalerite      -126.10 -171.28  -45.18  ZnS
      Spinel           -10.84   26.76   37.61  Al2MgO4
      Starkeyite        -4.72   -5.72   -1.00  MgSO4:4H2O
      Stilbite           2.22    3.03    0.81
Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
      Stilleite        -83.89 -174.13  -90.24  ZnSe
      Strengite         -5.82   -4.20    1.63  FePO4:2H2O
      Sylvite           -7.70   -6.87    0.83  KCl
      Syngenite         -5.97  -13.57   -7.60  K2Ca(SO4)2:H2O
      Tachyhydrite     -47.19  -30.05   17.14  Mg2CaCl6:12H2O
      Talc              -1.17   19.81   20.99  Mg3Si4O10(OH)2
      Tb               -158.69  -41.80  116.89  Tb
      Tb(OH)3             4.31   19.99   15.69  Tb(OH)3
      Tb(OH)3(am)         1.21   19.99   18.79  Tb(OH)3
      Tb2(CO3)3           9.24    6.02   -3.21  Tb2(CO3)3
      Tb2O3              -7.09   40.01   47.10  Tb2O3
      TbF3:.5H2O        -30.40  -47.10  -16.70  TbF3:.5H2O
      TbPO4:10H2O         9.07   -2.91  -11.98  TbPO4:10H2O
      Tc               -102.70 -159.62  -56.92  Tc
      Tc(OH)2           -63.82 -118.42  -54.61  Tc(OH)2
      Tc(OH)3           -50.20  -97.83  -47.62  Tc(OH)3
      Tc2O7             -43.93  -30.83   13.10  Tc2O7
      Tc2O7(g)          -52.18  -30.83   21.35  Tc2O7
      Tc2S7            -841.94-1308.17 -466.23  Tc2S7
      Tc3O4            -158.18 -314.05 -155.87  Tc3O4
```

Tc4O7	-181.31	-350.07	-168.76	Tc4O7
TcO2:2H2O(am)	-40.01	-77.23	-37.22	TcO2:2H2O
TcO3	-23.19	-36.01	-12.83	TcO3
TcOH	-82.54	-139.02	-56.48	TcOH
TcS2	-275.79	-442.17	-166.38	TcS2
TcS3	-373.14	-583.45	-210.30	TcS3
Tephroite	-21.40	1.63	23.02	Mn2SiO4
Thenardite	-2.62	-2.98	-0.36	Na2SO4
Thermonatrite	-7.58	3.36	10.94	Na2CO3:H2O
Tobermorite-11A	-23.82	41.57	65.39	Ca5Si6H11O22.5
Tobermorite-14A	-22.08	41.53	63.61	Ca5Si6H21O27.5
Tobermorite-9A	-27.27	41.58	68.86	Ca5Si6H6O20
Todorokite	-0.29	225.78	226.07	Mn7O12:3H2O
Tremolite	-6.96	53.96	60.93	Ca2Mg5Si8O22(OH)2
Tridymite	-0.19	-4.03	-3.84	SiO2
Troilite	-146.86	-184.41	-37.55	FeS
Trona-K	-18.29	-6.70	11.59	K2NaH(CO3)2:2H2O
Tyuyamunite	5.60	9.12	3.52	Ca(UO2)2(VO4)2
U	-204.60	-120.82	83.77	U
U(CO3)2	-59.55	-61.08	-1.53	U(CO3)2
U(g)	-290.15	-120.82	169.33	U
U(HPO4)2:4H2O	-42.18	-84.15	-41.98	U(HPO4)2:4H2O
U(OH)2SO4	-43.97	-56.10	-12.12	U(OH)2SO4
U(SO3)2	-117.59	-156.17	-38.58	U(SO3)2
U(SO4)2	-53.18	-73.76	-20.58	U(SO4)2
U(SO4)2:4H2O	-53.19	-73.79	-20.60	U(SO4)2:4H2O
U(SO4)2:8H2O	-52.20	-73.81	-21.62	U(SO4)2:8H2O
U2C3	-591.67	-522.84	68.84	U2C3
U2Cl10(g)	-227.08	-147.44	79.64	U2Cl10
U2Cl8(g)	-230.46	-166.28	64.17	U2Cl8
U2F10(g)	-243.88	-259.31	-15.44	U2F10
U2F9	-201.36	-257.55	-56.19	U2F9
U2O2Cl5	-120.80	-112.14	8.66	U2O2Cl5
U2O3F6	-126.11	-128.64	-2.53	U2O3F6
U2S3	-571.43	-665.47	-94.04	U2S3
U2Se3	-448.59	-674.02	-225.43	U2Se3
U3As4	-911.92	-924.78	-12.86	U3As4
U3O5F8	-167.71	-170.59	-2.88	U3O5F8
U3P4	-1070.70	-865.89	204.81	U3P4
U3S5	-891.49	-1068.85	-177.36	U3S5
U3Se4	-661.56	-938.96	-277.41	U3Se4
U3Se5	-691.94	-1083.09	-391.15	U3Se5
U4F17	-379.61	-513.32	-133.72	U4F17
U5O12Cl	-74.08	-100.27	-26.20	U5O12Cl
UAs	-269.22	-261.40	7.82	UAs
UAs2	-372.91	-401.98	-29.06	UAs2
UC	-259.15	-214.55	44.60	UC
UC1.94(alpha)	-328.75	-302.66	26.09	UC1.94
UCl(g)	-245.68	-111.40	134.28	UCl
UCl2(g)	-199.73	-101.98	97.75	UCl2
UCl2F2	-92.88	-105.52	-12.64	UCl2F2
UCl2I2	-134.96	-336.38	-201.41	UCl2I2

UCl3	-105.83	-92.56	13.27	UCl3
UCl3(g)	-151.44	-92.56	58.88	UCl3
UCl3F	-95.52	-94.33	1.19	UCl3F
UCl3I	-114.91	-209.76	-94.84	UCl3I
UCl4	-96.01	-83.14	12.87	UCl4
UCl4(g)	-120.44	-83.14	37.30	UCl4
UCl5	-109.47	-73.72	35.75	UCl5
UCl5(g)	-126.69	-73.72	52.97	UCl5
UCl6	-121.80	-64.30	57.50	UCl6
UCl6(g)	-127.67	-64.30	63.37	UCl6
UClF3	-90.07	-116.70	-26.64	UClF3
UClI3	-155.20	-462.99	-307.80	UClI3
UF(g)	-241.34	-122.59	118.76	UF
UF2(g)	-210.68	-124.36	86.32	UF2
UF3	-106.96	-126.12	-19.17	UF3
UF3(g)	-173.61	-126.12	47.49	UF3
UF4	-89.58	-127.89	-38.31	UF4
UF4(g)	-133.37	-127.89	5.48	UF4
UF4:2.5H2O	-85.41	-127.91	-42.49	UF4:2.5H2O
UF5(alpha)	-115.23	-129.66	-14.42	UF5
UF5(beta)	-114.91	-129.66	-14.75	UF5
UF5(g)	-134.46	-129.66	4.80	UF5
UF6	-148.73	-131.42	17.31	UF6
UF6(g)	-149.57	-131.42	18.15	UF6
UH3(beta)	-253.71	-182.63	71.07	UH3
UI(g)	-270.00	-238.02	31.98	UI
UI2(g)	-241.06	-355.22	-114.15	UI2
UI3	-167.71	-472.41	-304.71	UI3
UI3(g)	-214.31	-472.41	-258.11	UI3
UI4	-174.52	-589.61	-415.09	UI4
UI4(g)	-199.53	-589.61	-390.09	UI4
UN	-167.02	-234.94	-67.93	UN
UN1.59(alpha)	-159.46	-302.27	-142.81	UN1.59
UN1.73(alpha)	-157.98	-318.25	-160.27	UN1.73
UO(g)	-205.27	-79.62	125.65	UO
UO2(am)	-29.48	-38.42	-8.94	UO2
UO2(AsO3)2	-79.28	-72.37	6.91	UO2(AsO3)2
UO2(g)	-121.02	-38.42	82.60	UO2
UO2(IO3)2	-18.31	-25.61	-7.29	UO2(IO3)2
UO2(NO3)2	-31.40	-19.45	11.95	UO2(NO3)2
UO2(NO3)2:2H2O	-24.37	-19.46	4.91	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-23.15	-19.47	3.68	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-21.78	-19.49	2.29	UO2(NO3)2:6H2O
UO2(NO3)2:H2O	-27.96	-19.46	8.50	UO2(NO3)2:H2O
UO2(OH)2(beta)	-2.17	2.78	4.95	UO2(OH)2
UO2(PO3)2	-26.58	-42.92	-16.34	UO2(PO3)2
UO2.25	-18.02	-28.12	-10.10	UO2.25
UO2.25(beta)	-18.09	-28.12	-10.02	UO2.25
UO2.3333(beta)	-32.22	-49.37	-17.15	(UO2.3333)2
UO2.6667	-17.53	-21.90	-4.37	(UO2.6667)2
UO2Cl	-26.98	-29.00	-2.02	UO2Cl
UO2Cl2	-31.69	-19.58	12.11	UO2Cl2

UO2Cl2(g)	-67.51	-19.58	47.93	UO2Cl2
UO2Cl2:3H2O	-25.21	-19.60	5.61	UO2Cl2:3H2O
UO2Cl2:H2O	-27.87	-19.59	8.28	UO2Cl2:H2O
UO2ClOH:2H2O	-10.72	-8.41	2.30	UO2ClOH:2H2O
UO2CO3	-4.42	-8.55	-4.13	UO2CO3
UO2F2	-34.69	-41.95	-7.27	UO2F2
UO2F2(g)	-76.58	-41.95	34.63	UO2F2
UO2F2:3H2O	-34.59	-41.97	-7.38	UO2F2:3H2O
UO2FOH	-17.74	-19.59	-1.85	UO2FOH
UO2FOH:2H2O	-16.93	-19.60	-2.67	UO2FOH:2H2O
UO2FOH:H2O	-17.31	-19.60	-2.29	UO2FOH:H2O
UO2HPO4	-7.39	-20.07	-12.68	UO2HPO4
UO2HPO4:4H2O	-7.07	-20.10	-13.03	UO2HPO4:4H2O
UO2SO3	-43.72	-56.09	-12.37	UO2SO3
UO2SO4	-16.82	-14.89	1.93	UO2SO4
UO2SO4:2.5H2O	-13.40	-14.91	-1.50	UO2SO4:2.5H2O
UO2SO4:3.5H2O	-13.42	-14.91	-1.49	UO2SO4:3.5H2O
UO2SO4:3H2O	-13.50	-14.91	-1.41	UO2SO4:3H2O
UO2SO4:H2O	-8.83	-14.90	-6.07	UO2SO4:H2O
UO3(alpha)	-5.86	2.78	8.64	UO3
UO3(beta)	-5.53	2.78	8.31	UO3
UO3(g)	-68.17	2.78	70.95	UO3
UO3(gamma)	-4.93	2.78	7.71	UO3
UO3:.9H2O(alpha)	-2.24	2.78	5.02	UO3:.9H2O
UO3:2H2O	-2.07	2.77	4.84	UO3:2H2O
UOCl	-80.87	-70.20	10.67	UOCl
UOCl2	-57.15	-60.78	-3.63	UOCl2
UOCl3	-62.46	-51.36	11.10	UOCl3
UOF2	-55.95	-83.15	-27.20	UOF2
UOF2:H2O	-55.40	-83.16	-27.76	UOF2:H2O
UOF4	-91.25	-86.69	4.56	UOF4
UOF4(g)	-110.90	-86.69	24.21	UOF4
UOFOH	-42.81	-60.79	-17.98	UOFOH
UOFOH:.5H2O	-42.36	-60.79	-18.43	UOFOH:.5H2O
UP	-308.44	-246.68	61.76	UP
UP2	-453.82	-372.53	81.29	UP2
UP2O7	-42.00	-84.12	-42.12	UP2O7
UP2O7:20H2O	-46.57	-84.25	-37.68	UP2O7:20H2O
UPO5	-19.58	-40.67	-21.09	UPO5
Uraninite	-24.54	-38.42	-13.88	UO2
Uranium-selenide	-211.29	-264.95	-53.65	USe
Uranocircite	-12.66	-32.48	-19.82	Ba(UO2)2(PO4)2
Uranophane	-6.63	10.65	17.29	Ca(UO2)2(SiO3)2(OH)2
US	-253.83	-262.10	-8.27	US
US1.9	-315.71	-389.25	-73.53	US1.9
US2	-324.55	-403.37	-78.83	US2
US3	-426.84	-544.65	-117.81	US3
USe2(alpha)	-240.19	-409.07	-168.88	USe2
USe2(beta)	-240.04	-409.07	-169.03	USe2
USe3	-291.14	-553.20	-262.05	USe3
V	-127.54	-107.80	19.74	V
V2O4	-25.53	-50.80	-25.27	V2O4

V3O5	-68.50	-117.40	-48.91	V3O5
V4O7	-82.35	-142.80	-60.45	V4O7
Vivianite	-46.83	-51.55	-4.72	Fe3(PO4)2:8H2O
Wairakite	-6.10	11.82	17.92	CaAl2Si4O10(OH)4
Weeksite	-25.38	-10.01	15.38	K2(UO2)2(Si2O5)3:4H2O
Whitlockite	-1.92	-6.24	-4.32	Ca3(PO4)2
Witherite	-0.65	-3.67	-3.02	BaCO3
Wollastonite	-4.60	9.13	13.72	CaSiO3
Wurtzite	-128.40	-171.28	-42.88	ZnS
Wustite	-13.43	0.35	13.78	Fe.947O
Xonotlite	-36.99	54.75	91.74	Ca6Si6O17(OH)2
Yb	-154.73	-42.60	112.13	Yb
Yb(OH)3	4.51	19.19	14.69	Yb(OH)3
Yb(OH)3(am)	0.21	19.19	18.99	Yb(OH)3
Yb2(CO3)3	6.73	4.42	-2.31	Yb2(CO3)3
Yb2O3	-9.39	38.41	47.80	Yb2O3
YbF3:.5H2O	-31.90	-47.90	-16.00	YbF3:.5H2O
YbPO4:10H2O	8.07	-3.71	-11.78	YbPO4:10H2O
Zincite	-0.00	11.20	11.20	ZnO
Zn	-55.79	-30.00	25.79	Zn
Zn(BO2)2	1.59	9.90	8.31	Zn(BO2)2
Zn(ClO4)2:6H2O	-62.65	318.41	381.06	Zn(ClO4)2:6H2O
Zn(g)	-72.41	-30.00	42.41	Zn
Zn(IO3)2	-11.87	-17.19	-5.32	Zn(IO3)2
Zn(NO3)2:6H2O	-14.47	-11.07	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-0.74	11.19	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-0.47	11.19	11.66	Zn(OH)2
Zn(OH)2(gamma)	-0.69	11.19	11.88	Zn(OH)2
Zn2(OH)3Cl	-4.08	11.21	15.29	Zn2(OH)3Cl
Zn2SiO4	4.53	18.37	13.84	Zn2SiO4
Zn2SO4(OH)2	-2.86	4.72	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-50.86	-41.55	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-20.84	-1.75	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-8.93	33.74	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.24	-11.16	7.08	ZnCl2
ZnCl2(NH3)2	-136.17	-363.02	-226.85	ZnCl2(NH3)2
ZnCl2(NH3)4	-268.49	-714.89	-446.40	ZnCl2(NH3)4
ZnCl2(NH3)6	-402.47	-1066.75	-664.28	ZnCl2(NH3)6
ZnCO3:H2O	-0.28	-0.14	0.14	ZnCO3:H2O
ZnF2	-33.04	-33.54	-0.49	ZnF2
ZnI2	-49.13	-264.40	-215.27	ZnI2
ZnSeO3:H2O	-14.76	-50.53	-35.77	ZnSeO3:H2O
ZnSO4	-10.01	-6.47	3.53	ZnSO4
ZnSO4:6H2O	-4.81	-6.51	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.64	-6.52	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-5.93	-6.48	-0.55	ZnSO4:H2O
Zoisite	-6.74	36.40	43.14	Ca2Al3(SiO4)3OH

End of simulation.

```
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Reading input data for simulation 3.
-----------------------------------

-----------
```

End of run.

B-3 Sensitivity: Assume 20,000 gal/week of Applied Water Instead of 10,000 gal/week. Input File.

```
TITLE Rerun previous assemblage with a new mixing ratio
SOLUTION 1 Average Rainfall Composition
        units   mg/L
        pH      5.6
        pe      8.451
        temp    25.0
        redox   O(0)/O(-2)
        O(0)            1.0     O2(g) -0.7
Na    2
K     0.27
Ca    0.13
Mg    0.27
C     0.36
Cl    3.8
S(6)  0.62
SOLUTION 2 INEEL Water Quality (CPP-1, 6/6/91)
units  mg/L
pH    8
pe     8.4
redox   O(0)/O(-2)
        O(0)            1.0     O2(g) -0.7
C     194
Ca    54
Mg    14
Na    7.9
K     2.5
Cl    18
S(6)  22
MIX 1 Mixing Solutions 1 and 2
1   0.74
2   0.26
SAVE SOLUTION  3
END
USE SOLUTION  3
REACTION
NaCN  2.16e-04
NaI   9.49e-07
1.0
EQUILIBRIUM_PHASES 1
Calcite    0.0  6.1
```

```
Illite     0.0   4.1
Kaolinite  0.0  0.0
Quartz     0.0  106.5
Gypsum     0.0   0.0013
Albite     0.0  14.4
K-Feldspar  0.0  7.8
Fluorapatite  0.0  0.017
Dolomite  0.0   Enstatite  21.7
Yb2O3  0.0  0.0094
Fe(OH)3  0.0  2.89
Pyrite  0.0  0.17
Zincite  0.0  Sphalerite  0.05
Birnessite  0.0  0.008
Barite  0.0  0.022
Borax  0.0  0.07
PuO2   0.0  8.76e-09
CaUO4  0.0  0.000417
Ca2V2O7  0.0  0.0035
Tb2O3    0.0  0.03
TcO2:2H2O(am)   0.0  5.72e-08
Ca3(AsO4)2  0.0  0.0006
Niter  0.0  0.001
Halite    0.0  0.0009
CaSeO4    0.0  1.8e-04
O2(g)   -0.7   1.0
CO2(g)    -3.5   1.0
END
```

B-4 Sensitivity: Assume 20,000 gal/week of Applied Water Instead of 10,000 gal/week. Output File.

```
Input file: C:\Documents\INEEL\pqe2\EDF274_update2.pqi
  Output file: C:\Documents\INEEL\pqe2\EDF274_update2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive\llnl.dat

------------------
Reading data base.
------------------

      LLNL_AQUEOUS_MODEL_PARAMETERS
      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive\llnl.dat
      TITLE Rerun previous assemblage with a new mixing ratio
      SOLUTION 1 Average Rainfall Composition
              units   mg/L
              pH      5.6
              pe      8.451
              temp    25.0
              redox   O(0)/O(-2)
              O(0)            1.0     O2(g) -0.7
      Na    2
      K     0.27
      Ca    0.13
      Mg    0.27
      C     0.36
      Cl    3.8
      S(6)  0.62
      SOLUTION 2 INEEL Water Quality (CPP-1, 6/6/91)
      units  mg/L
      pH    8
      pe     8.4
      redox   O(0)/O(-2)
              O(0)            1.0     O2(g) -0.7
      C     194
      Ca    54
      Mg    14
```

```
      Na    7.9
      K     2.5
      Cl    18
      S(6)  22
      MIX 1 Mixing Solutions 1 and 2
      1   0.74
      2   0.26
      SAVE SOLUTION  3
      END
-----
TITLE
-----

 Rerun previous assemblage with a new mixing ratio

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.   Average Rainfall Composition

------------------Solution composition------------------------------

Elements           Molality       Moles

C                5.902e-006  5.902e-006
Ca               3.244e-006  3.244e-006
Cl               1.072e-004  1.072e-004
K                6.906e-006  6.906e-006
Mg               1.111e-005  1.111e-005
Na               8.700e-005  8.700e-005
O(0)             5.113e-004  5.113e-004  Equilibrium with O2(g)
S(6)             6.456e-006  6.456e-006

-----------------Description of solution----------------------------

                                       pH  =   5.600
                                       pe  =   8.451
                          Activity of water  =   1.000
                             Ionic strength  =  1.438e-004
                           Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  = -1.669e-006
                          Total CO2 (mol/kg)  =  5.902e-006
                        Temperature (deg C)  =  25.000
                   Electrical balance (eq)  =  4.179e-006
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   1.70
                                Iterations  =   4
                                   Total H  = 1.110507e+002
                                   Total O  = 5.552587e+001
```

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	15.0007	0.8874

----------Distribution of species----------

Species	Molality	Log Activity	Log Molality	Log Activity	Log Gamma
H+	2.546e-006	2.512e-006	-5.594	-5.600	-0.006
OH-	3.889e-009	3.836e-009	-8.410	-8.416	-0.006
H2O	5.553e+001	1.000e+000	-0.000	-0.000	0.000
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-266.969	-266.969	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-239.283	-239.283	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-148.571	-148.571	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-51.542	-51.542	0.000
C(4)	5.902e-006				
CO2	5.027e-006	5.027e-006	-5.299	-5.299	0.000
HCO3-	8.748e-007	8.627e-007	-6.058	-6.064	-0.006
MgHCO3+	1.067e-010	1.052e-010	-9.972	-9.978	-0.006
NaHCO3	1.059e-010	1.059e-010	-9.975	-9.975	0.000
CaHCO3+	3.179e-011	3.136e-011	-10.498	-10.504	-0.006
CO3-2	1.611e-011	1.524e-011	-10.793	-10.817	-0.024
MgCO3	1.692e-013	1.692e-013	-12.771	-12.771	0.000
CaCO3	1.083e-013	1.083e-013	-12.965	-12.965	0.000
NaCO3-	4.638e-015	4.574e-015	-14.334	-14.340	-0.006
Ca	3.244e-006				
Ca+2	3.241e-006	3.067e-006	-5.489	-5.513	-0.024
CaSO4	2.725e-009	2.725e-009	-8.565	-8.565	0.000
CaCl+	6.967e-011	6.871e-011	-10.157	-10.163	-0.006
CaHCO3+	3.179e-011	3.136e-011	-10.498	-10.504	-0.006
CaOH+	1.749e-013	1.725e-013	-12.757	-12.763	-0.006
CaCO3	1.083e-013	1.083e-013	-12.965	-12.965	0.000
CaCl2	8.542e-015	8.542e-015	-14.068	-14.068	0.000
Cl(-1)	1.072e-004				
Cl-	1.072e-004	1.057e-004	-3.970	-3.976	-0.006
NaCl	1.594e-009	1.594e-009	-8.798	-8.798	0.000
MgCl+	8.786e-010	8.665e-010	-9.056	-9.062	-0.006
CaCl+	6.967e-011	6.871e-011	-10.157	-10.163	-0.006
HCl	5.963e-011	5.963e-011	-10.225	-10.225	0.000
KCl	2.417e-011	2.417e-011	-10.617	-10.617	0.000
CaCl2	8.542e-015	8.542e-015	-14.068	-14.068	0.000
Cl(1)	1.233e-019				
HClO	1.219e-019	1.219e-019	-18.914	-18.914	0.000

ClO-	1.327e-021	1.309e-021	-20.877	-20.883	-0.006
Cl(3)	2.103e-031				
ClO2-	2.095e-031	2.066e-031	-30.679	-30.685	-0.006
HClO2	7.674e-034	7.674e-034	-33.115	-33.115	0.000
Cl(5)	2.354e-027				
ClO3-	2.354e-027	2.321e-027	-26.628	-26.634	-0.006
Cl(7)	1.320e-027				
ClO4-	1.320e-027	1.301e-027	-26.880	-26.886	-0.006
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-44.302	-44.302	0.000
K	6.906e-006				
K+	6.905e-006	6.810e-006	-5.161	-5.167	-0.006
KSO4-	3.390e-010	3.343e-010	-9.470	-9.476	-0.006
KCl	2.417e-011	2.417e-011	-10.617	-10.617	0.000
KOH	9.400e-015	9.400e-015	-14.027	-14.027	0.000
KHSO4	7.410e-016	7.410e-016	-15.130	-15.130	0.000
Mg	1.111e-005				
Mg+2	1.109e-005	1.050e-005	-4.955	-4.979	-0.024
MgSO4	1.706e-008	1.706e-008	-7.768	-7.768	0.000
MgCl+	8.786e-010	8.665e-010	-9.056	-9.062	-0.006
MgHCO3+	1.067e-010	1.052e-010	-9.972	-9.978	-0.006
MgCO3	1.692e-013	1.692e-013	-12.771	-12.771	0.000
Mg4(OH)4+4	6.773e-038	5.429e-038	-37.169	-37.265	-0.096
Na	8.700e-005				
Na+	8.699e-005	8.579e-005	-4.061	-4.067	-0.006
NaSO4-	3.496e-009	3.448e-009	-8.456	-8.462	-0.006
NaCl	1.594e-009	1.594e-009	-8.798	-8.798	0.000
NaHCO3	1.059e-010	1.059e-010	-9.975	-9.975	0.000
NaOH	5.677e-014	5.677e-014	-13.246	-13.246	0.000
NaCO3-	4.638e-015	4.574e-015	-14.334	-14.340	-0.006
O(0)	5.113e-004				
O2	2.556e-004	2.556e-004	-3.592	-3.592	0.000
S(6)	6.456e-006				
SO4-2	6.430e-006	6.083e-006	-5.192	-5.216	-0.024
MgSO4	1.706e-008	1.706e-008	-7.768	-7.768	0.000
NaSO4-	3.496e-009	3.448e-009	-8.456	-8.462	-0.006
CaSO4	2.725e-009	2.725e-009	-8.565	-8.565	0.000
HSO4-	1.565e-009	1.543e-009	-8.805	-8.812	-0.006
KSO4-	3.390e-010	3.343e-010	-9.470	-9.476	-0.006
KHSO4	7.410e-016	7.410e-016	-15.130	-15.130	0.000
H2SO4	3.658e-018	3.658e-018	-17.437	-17.437	0.000

----------Saturation indices----------

Phase	SI	log IAP	log KT	
Anhydrite	-6.38	-10.73	-4.35	CaSO4
Antarcticite	-17.56	-13.47	4.09	CaCl2:6H2O
Aphthitalite	-26.11	-30.00	-3.89	NaK3(SO4)2

Aragonite	-7.95	-5.98	1.97	CaCO3
Arcanite	-13.71	-15.55	-1.84	K2SO4
Artinite	-18.85	0.78	19.63	Mg2CO3(OH)2:3H2O
Bassanite	-7.02	-10.73	-3.71	CaSO4:0.5H2O
Bischofite	-17.32	-12.93	4.39	MgCl2:6H2O
Bloedite	-21.07	-23.54	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-10.06	6.22	16.28	Mg(OH)2
Burkeite	-44.78	-35.30	9.49	Na6CO3(SO4)2
C	-72.22	-8.07	64.15	C
C(g)	-189.84	-8.07	181.77	C
Ca	-132.35	7.48	139.83	Ca
Ca(g)	-157.59	7.48	165.07	Ca
Ca2Cl2(OH)2:H2O	-34.07	-7.78	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-64.73	3.59	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-7.80	-5.98	1.82	CaCO3
Carnallite	-26.35	-22.07	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-7.19	-10.73	-3.54	CaSO4:0.5H2O
CH4(g)	-145.73	-4.48	141.25	CH4
Chloromagnesite	-34.75	-12.93	21.82	MgCl2
Cl2(g)	-23.94	-20.95	2.99	Cl2
CO(g)	-48.54	-9.87	38.68	CO
CO2(g)	-3.84	-11.66	-7.83	CO2
Dolomite	-13.89	-11.42	2.47	CaMg(CO3)2
Dolomite-dis	-15.43	-11.42	4.01	CaMg(CO3)2
Dolomite-ord	-13.88	-11.42	2.46	CaMg(CO3)2
Epsomite	-8.23	-10.19	-1.96	MgSO4:7H2O
Gaylussite	-25.74	-14.57	11.16	CaNa2(CO3)2:5H2O
Glauberite	-18.61	-24.08	-5.47	Na2Ca(SO4)2
Gypsum	-6.20	-10.73	-4.53	CaSO4:2H2O
H2(g)	-41.20	1.80	43.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-9.61	-8.04	1.56	NaCl
HCl(g)	-15.88	-9.58	6.30	HCl
Hexahydrite	-8.47	-10.19	-1.73	MgSO4:6H2O
Huntite	-32.52	-22.31	10.22	CaMg3(CO3)4
Hydromagnesite	-46.29	-15.55	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-25.21	-13.47	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-69.65	1.33	70.98	K
K(g)	-80.25	1.33	81.58	K
K2CO3:1.5H2O	-24.18	-10.80	13.38	K2CO3:1.5H2O
K2O	-83.17	0.87	84.04	K2O
K3H(SO4)2	-27.91	-31.53	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-94.23	-66.52	27.71	K8H4(CO3)6:3H2O
Kainite	-19.03	-19.34	-0.31	KMgClSO4:3H2O
Kalicinite	-11.51	-11.23	0.28	KHCO3
Kieserite	-9.93	-10.19	-0.27	MgSO4:H2O
KMgCl3	-43.32	-22.07	21.25	KMgCl3
KMgCl3:2H2O	-36.04	-22.07	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-19.96	-9.70	10.26	KNaCO3:6H2O
Lansfordite	-10.28	-5.44	4.84	MgCO3:5H2O

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      Leonite          -21.63  -25.74   -4.11  K2Mg(SO4)2:4H2O
      Lime             -26.88    5.69   32.57  CaO
      Magnesite         -7.72   -5.44    2.27  MgCO3
      Mercallite       -14.54  -15.98   -1.44  KHSO4
      Mg               -114.50    8.02  122.52  Mg
      Mg(g)            -134.23    8.02  142.25  Mg
      Mg1.25SO4(OH)0.5:0.5H2O -13.83   -8.64    5.20
Mg1.25SO4(OH)0.5:0.5H2O
      Mg1.5SO4(OH)     -16.29   -7.08    9.21  Mg1.5SO4(OH)
      MgCl2:2H2O       -25.66  -12.93   12.73  MgCl2:2H2O
      MgCl2:4H2O       -20.23  -12.93    7.30  MgCl2:4H2O
      MgCl2:H2O        -29.00  -12.93   16.07  MgCl2:H2O
      MgOHCl           -19.25   -3.35   15.89  MgOHCl
      MgSO4            -15.02  -10.19    4.83  MgSO4
      Mirabilite       -12.19  -13.35   -1.15  Na2SO4:10H2O
      Misenite        -100.37 -111.45  -11.08  K8H6(SO4)7
      Monohydrocalcite  -8.66   -5.98    2.68  CaCO3:H2O
      Na               -64.94    2.43   67.37  Na
      Na(g)            -78.43    2.43   80.86  Na
      Na2CO3           -19.76   -8.60   11.16  Na2CO3
      Na2CO3:7H2O      -18.54   -8.60    9.94  Na2CO3:7H2O
      Na2O             -64.35    3.07   67.42  Na2O
      Na3H(SO4)2       -27.34  -28.23   -0.89  Na3H(SO4)2
      Na4Ca(SO4)3:2H2O -31.53  -37.43   -5.89  Na4Ca(SO4)3:2H2O
      Nahcolite         -9.99  -10.13   -0.14  NaHCO3
      Natron           -18.19   -8.60    9.59  Na2CO3:10H2O
      Nesquehonite     -10.73   -5.44    5.29  MgCO3:3H2O
      O2(g)             -0.70   -3.59   -2.89  O2
      Oxychloride-Mg   -22.97    2.87   25.83  Mg2Cl(OH)3:4H2O
      Pentahydrite      -8.81  -10.19   -1.39  MgSO4:5H2O
      Periclase        -15.10    6.22   21.33  MgO
      Picromerite      -21.30  -25.74   -4.44  K2Mg(SO4)2:6H2O
      Pirssonite       -25.90  -14.57   11.32  Na2Ca(CO3)2:2H2O
      Polyhalite       -32.89  -47.20  -14.31  K2MgCa2(SO4)4:2H2O
      Portlandite      -16.86    5.69   22.55  Ca(OH)2
      Starkeyite        -9.19  -10.19   -1.00  MgSO4:4H2O
      Sylvite           -9.97   -9.14    0.83  KCl
      Syngenite        -18.68  -26.28   -7.60  K2Ca(SO4)2:H2O
      Tachyhydrite     -56.47  -39.33   17.14  Mg2CaCl6:12H2O
      Thenardite       -12.99  -13.35   -0.36  Na2SO4


      Thermonatrite    -19.53   -8.60   10.94  Na2CO3:H2O
      Trona-K          -32.52  -20.93   11.59  K2NaH(CO3)2:2H2O

Initial solution 2.   INEEL Water Quality (CPP-1, 6/6/91)

------------------Solution composition------------------------------

Elements           Molality       Moles

C                3.181e-003  3.181e-003
```

Ca	1.348e-003	1.348e-003	
Cl	5.079e-004	5.079e-004	
K	6.396e-005	6.396e-005	
Mg	5.762e-004	5.762e-004	
Na	3.437e-004	3.437e-004	
O(0)	5.105e-004	5.105e-004	Equilibrium with O2(g)
S(6)	2.291e-004	2.291e-004	

----------Description of solution----------

pH	= 8.000
pe	= 8.400
Activity of water	= 1.000
Ionic strength	= 6.037e-003
Mass of water (kg)	= 1.000e+000
Total alkalinity (eq/kg)	= 3.167e-003
Total CO2 (mol/kg)	= 3.181e-003
Temperature (deg C)	= 25.000
Electrical balance (eq)	= 1.228e-004
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 1.53
Iterations	= 5
Total H	= 1.110537e+002
Total O	= 5.553623e+001

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	12.6007	0.7454

----------Distribution of species----------

Species	Molality	Log Activity	Log Molality	Log Activity	Log Gamma
OH-	1.047e-006	9.634e-007	-5.980	-6.016	-0.036
H+	1.077e-008	1.000e-008	-7.968	-8.000	-0.032
H2O	5.553e+001	9.999e-001	-0.000	-0.000	0.000
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-264.752	-264.752	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-237.066	-237.066	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-147.463	-147.463	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-50.433	-50.433	0.000
C(4)	3.181e-003				
HCO3-	3.020e-003	2.781e-003	-2.520	-2.556	-0.036
CO2	6.441e-005	6.451e-005	-4.191	-4.190	0.001
CaHCO3+	3.309e-005	3.047e-005	-4.480	-4.516	-0.036
CaCO3	2.644e-005	2.644e-005	-4.578	-4.578	0.000
CO3-2	1.712e-005	1.234e-005	-4.766	-4.909	-0.142

MgHCO3+	1.403e-005	1.292e-005	-4.853	-4.889	-0.036
MgCO3	5.221e-006	5.221e-006	-5.282	-5.282	0.000
NaHCO3	1.253e-006	1.253e-006	-5.902	-5.902	0.000
NaCO3-	1.477e-008	1.360e-008	-7.831	-7.866	-0.036
Ca	1.348e-003				
Ca+2	1.269e-003	9.247e-004	-2.896	-3.034	-0.138
CaHCO3+	3.309e-005	3.047e-005	-4.480	-4.516	-0.036
CaCO3	2.644e-005	2.644e-005	-4.578	-4.578	0.000
CaSO4	1.890e-005	1.890e-005	-4.724	-4.724	0.000
CaCl+	9.928e-008	9.143e-008	-7.003	-7.039	-0.036
CaOH+	1.418e-008	1.306e-008	-7.848	-7.884	-0.036
CaCl2	5.017e-011	5.017e-011	-10.300	-10.300	0.000
Cl(-1)	5.079e-004				
Cl-	5.076e-004	4.665e-004	-3.294	-3.331	-0.037
MgCl+	1.582e-007	1.457e-007	-6.801	-6.837	-0.036
CaCl+	9.928e-008	9.143e-008	-7.003	-7.039	-0.036
NaCl	2.583e-008	2.583e-008	-7.588	-7.588	0.000
KCl	9.198e-010	9.198e-010	-9.036	-9.036	0.000
CaCl2	5.017e-011	5.017e-011	-10.300	-10.300	0.000
HCl	1.048e-012	1.048e-012	-11.980	-11.980	0.000
Cl(1)	8.416e-021				
ClO-	6.274e-021	5.777e-021	-20.202	-20.238	-0.036
HClO	2.143e-021	2.143e-021	-20.669	-20.669	0.000
Cl(3)	9.904e-031				
ClO2-	9.904e-031	9.120e-031	-30.004	-30.040	-0.036
HClO2	1.348e-035	1.348e-035	-34.870	-34.870	0.000
Cl(5)	1.114e-026				
ClO3-	1.114e-026	1.024e-026	-25.953	-25.990	-0.036
Cl(7)	6.244e-027				
ClO4-	6.244e-027	5.744e-027	-26.205	-26.241	-0.036
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-44.302	-44.302	0.001
K	6.396e-005				
K+	6.389e-005	5.872e-005	-4.195	-4.231	-0.037
KSO4-	7.201e-008	6.631e-008	-7.143	-7.178	-0.036
KCl	9.198e-010	9.198e-010	-9.036	-9.036	0.000
KOH	2.036e-011	2.036e-011	-10.691	-10.691	0.000
KHSO4	5.851e-016	5.851e-016	-15.233	-15.233	0.000
Mg	5.762e-004				
Mg+2	5.418e-004	4.001e-004	-3.266	-3.398	-0.132
MgSO4	1.495e-005	1.495e-005	-4.825	-4.825	0.000
MgHCO3+	1.403e-005	1.292e-005	-4.853	-4.889	-0.036
MgCO3	5.221e-006	5.221e-006	-5.282	-5.282	0.000
MgCl+	1.582e-007	1.457e-007	-6.801	-6.837	-0.036
Mg4(OH)4+4	1.643e-021	4.554e-022	-20.784	-21.342	-0.557
Na	3.437e-004				
Na+	3.421e-004	3.151e-004	-3.466	-3.502	-0.036
NaHCO3	1.253e-006	1.253e-006	-5.902	-5.902	0.000
NaSO4-	3.163e-007	2.912e-007	-6.500	-6.536	-0.036
NaCl	2.583e-008	2.583e-008	-7.588	-7.588	0.000

NaCO3-	1.477e-008	1.360e-008	-7.831	-7.866	-0.036
NaOH	5.236e-011	5.236e-011	-10.281	-10.281	0.000
O(0)	5.105e-004				
O2	2.553e-004	2.556e-004	-3.593	-3.592	0.001
S(6)	2.291e-004				
SO4-2	1.949e-004	1.399e-004	-3.710	-3.854	-0.144
CaSO4	1.890e-005	1.890e-005	-4.724	-4.724	0.000
MgSO4	1.495e-005	1.495e-005	-4.825	-4.825	0.000
NaSO4-	3.163e-007	2.912e-007	-6.500	-6.536	-0.036
KSO4-	7.201e-008	6.631e-008	-7.143	-7.178	-0.036
HSO4-	1.535e-010	1.413e-010	-9.814	-9.850	-0.036
KHSO4	5.851e-016	5.851e-016	-15.233	-15.233	0.000
H2SO4	1.333e-021	1.333e-021	-20.875	-20.875	0.000

----------Saturation indices----------

Phase	SI	log IAP	log KT	
Anhydrite	-2.54	-6.89	-4.35	CaSO4
Antarcticite	-13.79	-9.70	4.09	CaCl2:6H2O
Aphthitalite	-20.02	-23.90	-3.89	NaK3(SO4)2
Aragonite	0.44	2.41	1.97	CaCO3
Arcanite	-10.47	-12.32	-1.84	K2SO4
Artinite	-4.98	14.65	19.63	Mg2CO3(OH)2:3H2O
Bassanite	-3.18	-6.89	-3.71	CaSO4:0.5H2O
Bischofite	-14.45	-10.06	4.39	MgCl2:6H2O
Bloedite	-15.63	-18.11	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-3.68	12.60	16.28	Mg(OH)2
Burkeite	-32.76	-23.27	9.49	Na6CO3(SO4)2
C	-71.11	-6.96	64.15	C
C(g)	-188.73	-6.96	181.77	C
Ca	-125.07	14.76	139.83	Ca
Ca(g)	-150.31	14.76	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.02	3.27	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-39.13	29.20	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.59	2.41	1.82	CaCO3
Carnallite	-21.89	-17.62	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-3.35	-6.89	-3.54	CaSO4:0.5H2O
CH4(g)	-144.62	-3.37	141.25	CH4
Chloromagnesite	-31.88	-10.06	21.82	MgCl2
Cl2(g)	-27.45	-24.46	2.99	Cl2
CO(g)	-47.44	-8.76	38.68	CO
CO2(g)	-2.73	-10.56	-7.83	CO2
Dolomite	1.98	4.46	2.47	CaMg(CO3)2
Dolomite-dis	0.44	4.46	4.01	CaMg(CO3)2
Dolomite-ord	1.99	4.46	2.46	CaMg(CO3)2
Epsomite	-5.29	-7.25	-1.96	MgSO4:7H2O
Gaylussite	-10.31	0.85	11.16	CaNa2(CO3)2:5H2O
Glauberite	-12.28	-17.75	-5.47	Na2Ca(SO4)2
Gypsum	-2.36	-6.89	-4.53	CaSO4:2H2O
H2(g)	-41.20	1.80	43.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O

Halite	-8.40	-6.83	1.56	NaCl
HCl(g)	-17.63	-11.33	6.30	HCl
Hexahydrite	-5.53	-7.25	-1.73	MgSO4:6H2O
Huntite	-1.67	8.55	10.22	CaMg3(CO3)4
Hydromagnesite	-9.95	20.79	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.44	-9.70	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-66.31	4.67	70.98	K
K(g)	-76.91	4.67	81.58	K
K2CO3:1.5H2O	-16.40	-3.02	13.38	K2CO3:1.5H2O
K2O	-76.50	7.54	84.04	K2O
K3H(SO4)2	-24.78	-28.40	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-60.89	-33.19	27.71	K8H4(CO3)6:3H2O
Kainite	-14.50	-14.81	-0.31	KMgClSO4:3H2O
Kalicinite	-7.07	-6.79	0.28	KHCO3
Kieserite	-6.99	-7.25	-0.27	MgSO4:H2O
KMgCl3	-38.87	-17.62	21.25	KMgCl3
KMgCl3:2H2O	-31.58	-17.62	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-12.55	-2.29	10.26	KNaCO3:6H2O
Lansfordite	-2.79	2.05	4.84	MgCO3:5H2O
Leonite	-15.46	-19.57	-4.11	K2Mg(SO4)2:4H2O
Lime	-19.60	12.97	32.57	CaO
Magnesite	-0.23	2.05	2.27	MgCO3
Mercallite	-14.65	-16.09	-1.44	KHSO4
Mg	-108.12	14.40	122.52	Mg
Mg(g)	-127.85	14.40	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-9.30	-4.10	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-10.16	-0.95	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.79	-10.06	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.36	-10.06	7.30	MgCl2:4H2O
MgCl2:H2O	-26.13	-10.06	16.07	MgCl2:H2O
MgOHCl	-14.62	1.27	15.89	MgOHCl
MgSO4	-12.08	-7.25	4.83	MgSO4
Mirabilite	-9.70	-10.86	-1.15	Na2SO4:10H2O
Misenite	-97.75	-108.83	-11.08	K8H6(SO4)7
Monohydrocalcite	-0.27	2.41	2.68	CaCO3:H2O
Na	-61.97	5.40	67.37	Na
Na(g)	-75.46	5.40	80.86	Na
Na2CO3	-12.72	-1.56	11.16	Na2CO3
Na2CO3:7H2O	-11.50	-1.56	9.94	Na2CO3:7H2O
Na2O	-58.42	9.00	67.42	Na2O
Na3H(SO4)2	-25.32	-26.21	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-22.71	-28.60	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-5.92	-6.06	-0.14	NaHCO3
Natron	-11.15	-1.56	9.59	Na2CO3:10H2O
Nesquehonite	-3.24	2.05	5.29	MgCO3:3H2O
O2(g)	-0.70	-3.59	-2.89	O2
Oxychloride-Mg	-11.96	13.87	25.83	Mg2Cl(OH)3:4H2O
Pentahydrite	-5.87	-7.25	-1.39	MgSO4:5H2O
Periclase	-8.72	12.60	21.33	MgO

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      Picromerite     -15.13  -19.57   -4.44  K2Mg(SO4)2:6H2O
      Pirssonite      -10.47    0.85   11.32  Na2Ca(CO3)2:2H2O
      Polyhalite      -19.03  -33.35  -14.31  K2MgCa2(SO4)4:2H2O
      Portlandite      -9.58   12.97   22.55  Ca(OH)2
      Starkeyite       -6.25   -7.25   -1.00  MgSO4:4H2O
      Sylvite          -8.39   -7.56    0.83  KCl
      Syngenite       -11.60  -19.20   -7.60  K2Ca(SO4)2:H2O
      Tachyhydrite    -46.96  -29.82   17.14  Mg2CaCl6:12H2O
      Thenardite      -10.50  -10.86   -0.36  Na2SO4
      Thermonatrite   -12.50   -1.56   10.94  Na2CO3:H2O
      Trona-K         -20.66   -9.08   11.59  K2NaH(CO3)2:2H2O

-----------------------------------------
Beginning of batch-reaction calculations.
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Reaction step 1.

Using mix 1.    Mixing Solutions 1 and 2

Mixture 1. Mixing Solutions 1 and 2

      7.400e-001 Solution 1     Average Rainfall Composition
      2.600e-001 Solution 2     INEEL Water Quality (CPP-1, 6/6/91)
------------------Solution composition------------------------------

      Elements           Molality       Moles

      C                8.315e-004  8.315e-004
      Ca               3.528e-004  3.528e-004
      Cl               2.114e-004  2.114e-004
      K                2.174e-005  2.174e-005
      Mg               1.580e-004  1.580e-004
      Na               1.537e-004  1.537e-004
      S                6.435e-005  6.435e-005

-----------------Description of solution---------------------------

                                       pH  =   8.009  Charge balance
                                       pe  =  12.591  Adjusted to
redox equilibrium
                         Activity of water  =  1.000
                            Ionic strength  =  1.727e-003
                        Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  8.221e-004
                       Total CO2 (mol/kg)  =  8.315e-004
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  3.502e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  1.51
                                 Iterations  =  24
                                    Total H  = 1.110515e+002
                                    Total O  = 5.552857e+001
```

----------Distribution of species----------

Species	Molality	Log Activity	Molality	Log Activity	Log Gamma
OH-	1.031e-006	9.845e-007	-5.987	-6.007	-0.020
H+	1.022e-008	9.786e-009	-7.991	-8.009	-0.019
H2O	5.553e+001	1.000e+000	-0.000	-0.000	0.000
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-265.890	-265.890	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-238.204	-238.204	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-148.032	-148.032	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-51.002	-51.002	0.000
C(4)	8.315e-004				
HCO3-	8.030e-004	7.667e-004	-3.095	-3.115	-0.020
CO2	1.740e-005	1.740e-005	-4.760	-4.759	0.000
CO3-2	4.179e-006	3.476e-006	-5.379	-5.459	-0.080
CaHCO3+	2.745e-006	2.621e-006	-5.561	-5.582	-0.020
CaCO3	2.324e-006	2.324e-006	-5.634	-5.634	0.000
MgHCO3+	1.209e-006	1.154e-006	-5.918	-5.938	-0.020
MgCO3	4.765e-007	4.765e-007	-6.322	-6.322	0.000
NaHCO3	1.608e-007	1.608e-007	-6.794	-6.794	0.000
NaCO3-	1.867e-009	1.783e-009	-8.729	-8.749	-0.020
Ca	3.528e-004				
Ca+2	3.456e-004	2.885e-004	-3.461	-3.540	-0.078
CaHCO3+	2.745e-006	2.621e-006	-5.561	-5.582	-0.020
CaCO3	2.324e-006	2.324e-006	-5.634	-5.634	0.000
CaSO4	2.116e-006	2.116e-006	-5.675	-5.675	0.000
CaCl+	1.291e-008	1.233e-008	-7.889	-7.909	-0.020
CaOH+	4.361e-009	4.164e-009	-8.360	-8.381	-0.020
CaCl2	2.924e-012	2.924e-012	-11.534	-11.534	0.000
Cl(-1)	2.114e-004				
Cl-	2.113e-004	2.017e-004	-3.675	-3.695	-0.020
MgCl+	2.137e-008	2.040e-008	-7.670	-7.690	-0.020
CaCl+	1.291e-008	1.233e-008	-7.889	-7.909	-0.020
NaCl	5.196e-009	5.196e-009	-8.284	-8.284	0.000
KCl	1.404e-010	1.404e-010	-9.853	-9.853	0.000
CaCl2	2.924e-012	2.924e-012	-11.534	-11.534	0.000
HCl	4.432e-013	4.432e-013	-12.353	-12.353	0.000
Cl(1)	3.522e-021				
ClO-	2.616e-021	2.497e-021	-20.582	-20.603	-0.020
HClO	9.063e-022	9.063e-022	-21.043	-21.043	0.000
Cl(3)	4.129e-031				
ClO2-	4.129e-031	3.942e-031	-30.384	-30.404	-0.020
HClO2	5.704e-036	5.704e-036	-35.244	-35.244	0.000
Cl(5)	4.639e-027				
ClO3-	4.639e-027	4.428e-027	-26.334	-26.354	-0.020

Cl(7)	2.601e-027				
ClO4-	2.601e-027	2.483e-027	-26.585	-26.605	-0.020
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-44.302	-44.302	0.000
K	2.174e-005				
K+	2.173e-005	2.074e-005	-4.663	-4.683	-0.020
KSO4-	8.802e-009	8.404e-009	-8.055	-8.076	-0.020
KCl	1.404e-010	1.404e-010	-9.853	-9.853	0.000
KOH	7.347e-012	7.347e-012	-11.134	-11.134	0.000
KHSO4	7.256e-017	7.256e-017	-16.139	-16.139	0.000
Mg	1.580e-004				
Mg+2	1.546e-004	1.296e-004	-3.811	-3.887	-0.077
MgSO4	1.738e-006	1.738e-006	-5.760	-5.760	0.000
MgHCO3+	1.209e-006	1.154e-006	-5.918	-5.938	-0.020
MgCO3	4.765e-007	4.765e-007	-6.322	-6.322	0.000
MgCl+	2.137e-008	2.040e-008	-7.670	-7.690	-0.020
Mg4(OH)4+4	1.133e-023	5.470e-024	-22.946	-23.262	-0.316
Na	1.537e-004				
Na+	1.535e-004	1.466e-004	-3.814	-3.834	-0.020
NaHCO3	1.608e-007	1.608e-007	-6.794	-6.794	0.000
NaSO4-	5.093e-008	4.863e-008	-7.293	-7.313	-0.020
NaCl	5.196e-009	5.196e-009	-8.284	-8.284	0.000
NaCO3-	1.867e-009	1.783e-009	-8.729	-8.749	-0.020
NaOH	2.490e-011	2.490e-011	-10.604	-10.604	0.000
O(0)	5.111e-004				
O2	2.555e-004	2.557e-004	-3.593	-3.592	0.000
S3O6-2	0.000e+000	0.000e+000	-183.662	-183.742	-0.081
S2-2	0.000e+000	0.000e+000	-255.271	-255.352	-0.081
S4O6-2	0.000e+000	0.000e+000	-277.309	-277.389	-0.081
S3-2	0.000e+000	0.000e+000	-362.341	-362.421	-0.081
S5O6-2	0.000e+000	0.000e+000	-399.835	-399.916	-0.081
S4-2	0.000e+000	0.000e+000	-469.638	-469.718	-0.081
S5-2	0.000e+000	0.000e+000	-577.151	-577.232	-0.081
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-143.386	-143.406	-0.020
H2S	0.000e+000	0.000e+000	-144.406	-144.406	0.000
S-2	0.000e+000	0.000e+000	-148.244	-148.323	-0.080
S2-2	0.000e+000	0.000e+000	-255.271	-255.352	-0.081
S3-2	0.000e+000	0.000e+000	-362.341	-362.421	-0.081
S4-2	0.000e+000	0.000e+000	-469.638	-469.718	-0.081
S5-2	0.000e+000	0.000e+000	-577.151	-577.232	-0.081
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-150.826	-150.906	-0.081
HS2O3-	0.000e+000	0.000e+000	-157.882	-157.902	-0.020
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-140.048	-140.127	-0.080
S(4)	0.000e+000				
SO3-2	0.000e+000	0.000e+000	-49.041	-49.121	-0.080
HSO3-	0.000e+000	0.000e+000	-49.879	-49.899	-0.020
H2SO3	0.000e+000	0.000e+000	-55.926	-55.926	0.000
SO2	0.000e+000	0.000e+000	-56.027	-56.027	0.000

S2O5-2	0.000e+000	0.000e+000	-104.547	-104.628	-0.081
S3O6-2	0.000e+000	0.000e+000	-183.662	-183.742	-0.081
S4O6-2	0.000e+000	0.000e+000	-277.309	-277.389	-0.081
S5O6-2	0.000e+000	0.000e+000	-399.835	-399.916	-0.081
S(5)	0.000e+000				
S2O6-2	0.000e+000	0.000e+000	-74.109	-74.190	-0.081
S(6)	6.435e-005				
SO4-2	6.044e-005	5.021e-005	-4.219	-4.299	-0.081
CaSO4	2.116e-006	2.116e-006	-5.675	-5.675	0.000
MgSO4	1.738e-006	1.738e-006	-5.760	-5.760	0.000
NaSO4-	5.093e-008	4.863e-008	-7.293	-7.313	-0.020
KSO4-	8.802e-009	8.404e-009	-8.055	-8.076	-0.020
HSO4-	5.198e-011	4.963e-011	-10.284	-10.304	-0.020
KHSO4	7.256e-017	7.256e-017	-16.139	-16.139	0.000
H2SO4	4.583e-022	4.583e-022	-21.339	-21.339	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-48.788	-48.868	-0.081
S(8)	4.515e-032				
HSO5-	4.515e-032	4.311e-032	-31.345	-31.365	-0.020

-------------------Saturation indices-------------------------------

Phase	SI	log IAP	log KT	
Anhydrite	-3.49	-7.84	-4.35	CaSO4
Antarcticite	-15.02	-10.93	4.09	CaCl2:6H2O
Aphthitalite	-22.59	-26.48	-3.89	NaK3(SO4)2
Aragonite	-0.62	1.35	1.97	CaCO3
Arcanite	-11.82	-13.67	-1.84	K2SO4
Artinite	-6.49	13.14	19.63	Mg2CO3(OH)2:3H2O
Bassanite	-4.13	-7.84	-3.71	CaSO4:0.5H2O
Bischofite	-15.67	-11.28	4.39	MgCl2:6H2O
Bloedite	-17.68	-20.15	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-4.15	12.13	16.28	Mg(OH)2
Burkeite	-36.19	-26.71	9.49	Na6CO3(SO4)2
C	-71.68	-93.53	-21.85	C
C(g)	-189.30	-93.53	95.77	C
Ca	-125.56	-28.72	96.83	Ca
Ca(g)	-150.80	-28.72	122.07	Ca
Ca2Cl2(OH)2:H2O	-24.74	1.55	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-41.82	26.51	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-0.47	1.35	1.82	CaCO3
Carnallite	-23.93	-19.66	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-4.30	-7.84	-3.54	CaSO4:0.5H2O
CH4(g)	-145.19	-175.93	-30.74	CH4
Chloromagnesite	-33.09	-11.28	21.82	MgCl2
Cl2(g)	-28.20	17.79	45.99	Cl2
CO(g)	-48.01	-52.33	-4.32	CO
CO2(g)	-3.30	-11.12	-7.83	CO2
Dolomite	-0.11	2.36	2.47	CaMg(CO3)2
Dolomite-dis	-1.65	2.36	4.01	CaMg(CO3)2
Dolomite-ord	-0.10	2.36	2.46	CaMg(CO3)2
Epsomite	-6.22	-8.19	-1.96	MgSO4:7H2O

Gaylussite	-12.58	-1.42	11.16	CaNa2(CO3)2:5H2O
Glauberite	-14.34	-19.81	-5.47	Na2Ca(SO4)2
Gypsum	-3.31	-7.84	-4.53	CaSO4:2H2O
H2(g)	-41.20	-41.20	-0.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-143.42	-185.12	-41.70	H2S
Halite	-9.09	-7.53	1.56	NaCl
HCl(g)	-18.01	-11.70	6.30	HCl
Hexahydrite	-6.46	-8.19	-1.73	MgSO4:6H2O
Huntite	-5.84	4.37	10.22	CaMg3(CO3)4
Hydromagnesite	-14.58	16.16	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-22.68	-10.93	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-66.75	-17.27	49.48	K
K(g)	-77.35	-17.27	60.08	K
K2CO3:1.5H2O	-17.85	-4.47	13.38	K2CO3:1.5H2O
K2O	-77.38	6.65	84.04	K2O
K3H(SO4)2	-27.03	-30.66	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-67.85	-40.14	27.71	K8H4(CO3)6:3H2O
Kainite	-16.25	-16.57	-0.31	KMgClSO4:3H2O
Kalicinite	-8.08	-7.80	0.28	KHCO3
Kieserite	-7.92	-8.19	-0.27	MgSO4:H2O
KMgCl3	-40.90	-19.66	21.25	KMgCl3
KMgCl3:2H2O	-33.62	-19.66	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-13.88	-3.62	10.26	KNaCO3:6H2O
Lansfordite	-3.83	1.01	4.84	MgCO3:5H2O
Leonite	-17.74	-21.85	-4.11	K2Mg(SO4)2:4H2O
Lime	-20.09	12.48	32.57	CaO
Magnesite	-1.27	1.01	2.27	MgCO3
Mercallite	-15.55	-16.99	-1.44	KHSO4
Mg	-108.59	-29.07	79.52	Mg
Mg(g)	-128.32	-29.07	99.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.35	-5.15	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-11.33	-2.12	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-24.01	-11.28	12.73	MgCl2:2H2O
MgCl2:4H2O	-18.58	-11.28	7.30	MgCl2:4H2O
MgCl2:H2O	-27.35	-11.28	16.07	MgCl2:H2O
MgOHCl	-15.46	0.43	15.89	MgOHCl
MgSO4	-13.01	-8.19	4.83	MgSO4
Mirabilite	-10.81	-11.97	-1.15	Na2SO4:10H2O
Misenite	-104.54	-115.62	-11.08	K8H6(SO4)7
Monohydrocalcite	-1.32	1.35	2.68	CaCO3:H2O
Na	-62.30	-16.43	45.87	Na
Na(g)	-75.79	-16.43	59.36	Na
Na2CO3	-13.94	-2.77	11.16	Na2CO3
Na2CO3:7H2O	-12.71	-2.77	9.94	Na2CO3:7H2O
Na2O	-59.07	8.35	67.42	Na2O
Na3H(SO4)2	-27.22	-28.11	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-25.88	-31.77	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.81	-6.95	-0.14	NaHCO3
Natron	-12.36	-2.77	9.59	Na2CO3:10H2O

```
      Nesquehonite     -4.28    1.01    5.29  MgCO3:3H2O
      O2(g)            -0.70   82.40   83.10  O2
      Oxychloride-Mg  -13.27   12.56   25.83  Mg2Cl(OH)3:4H2O
      Pentahydrite     -6.80   -8.19   -1.39  MgSO4:5H2O
      Periclase        -9.19   12.13   21.33  MgO
      Picromerite     -17.41  -21.85   -4.44  K2Mg(SO4)2:6H2O
      Pirssonite      -12.74   -1.42   11.32  Na2Ca(CO3)2:2H2O
      Polyhalite      -23.22  -37.53  -14.31  K2MgCa2(SO4)4:2H2O
      Portlandite     -10.07   12.48   22.55  Ca(OH)2
      S              -108.10 -143.92  -35.82  S
      S2(g)          -230.10 -287.84  -57.75  S2
      SO2(g)          -56.20  -61.52   -5.32  SO2
      Starkeyite       -7.19   -8.19   -1.00  MgSO4:4H2O
      Sylvite          -9.21   -8.38    0.83  KCl
      Syngenite       -13.90  -21.50   -7.60  K2Ca(SO4)2:H2O
      Tachyhydrite    -50.63  -33.49   17.14  Mg2CaCl6:12H2O
      Thenardite      -11.61  -11.97   -0.36  Na2SO4
      Thermonatrite   -13.71   -2.77   10.94  Na2CO3:H2O
      Trona-K         -23.01  -11.42   11.59  K2NaH(CO3)2:2H2O

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

      USE SOLUTION  3

      REACTION
      NaCN  2.16e-04
      NaI   9.49e-07
      1.0
      EQUILIBRIUM_PHASES 1
      Calcite    0.0  6.1
      Illite     0.0   4.1
      Kaolinite  0.0  0.0
      Quartz     0.0  106.5
      Gypsum     0.0   0.0013
      Albite     0.0  14.4
      K-Feldspar  0.0  7.8
      Fluorapatite  0.0  0.017
      Dolomite  0.0   Enstatite  21.7
      Yb2O3  0.0  0.0094
      Fe(OH)3  0.0  2.89
      Pyrite  0.0  0.17
      Zincite  0.0  Sphalerite  0.05
      Birnessite  0.0  0.008
      Barite  0.0  0.022
      Borax  0.0  0.07
      PuO2   0.0  8.76e-09
      CaUO4  0.0  0.000417
```

```
      Ca2V2O7  0.0  0.0035
      Tb2O3    0.0  0.03
      TcO2:2H2O(am)   0.0  5.72e-08
      Ca3(AsO4)2  0.0  0.0006
      Niter  0.0  0.001
      Halite    0.0  0.0009
      CaSeO4    0.0  1.8e-04
      O2(g)   -0.7   1.0
      CO2(g)    -3.5   1.0
      END
-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 3.     Solution after simulation 1.
Using pure phase assemblage 1.
Using reaction 1.

Reaction 1.     Irreversible reaction defined in simulation 2.

       1.000e+000 moles of the following reaction have been added:

                    Relative
      Reactant         moles

      NaCN              0.00
      NaI               0.00

                    Relative
      Element          moles
      C                 0.00
      I                 0.00
      N                 0.00
      Na                0.00

--------------------Phase assemblage--------------------------------

                                                      Moles in assemblage
Phase            SI log IAP  log KT    Initial      Final      Delta

Albite         0.00    2.66    2.66 1.440e+001 1.418e+001 -2.237e-001
Barite         0.00  -10.01  -10.01 2.200e-002 2.200e-002 -1.923e-008
Birnessite     0.00  269.79  269.79 8.000e-003 8.000e-003 -7.118e-014
Borax         -0.00   12.04   12.04 7.000e-002 1.221e-002 -5.779e-002
Ca2V2O7       -0.47   16.71   17.18 3.500e-003             -3.500e-003
Ca3(AsO4)2   -53.49  -35.69   17.80 6.000e-004             -6.000e-004
Calcite       -0.00    1.82    1.82 6.100e+000 5.975e+000 -1.252e-001
CaSeO4        -4.28   -7.37   -3.09 1.800e-004             -1.800e-004
CaUO4          0.00   15.94   15.94 4.170e-004 4.136e-004 -3.406e-006
CO2(g)        -3.50  -11.33   -7.83 1.000e+000 1.063e+000  6.339e-002
```

Dolomite	-0.00	2.47	2.47			
MgSiO3	is reactant		2.170e+001	2.272e+001	1.024e+000	
Fe(OH)3	0.00	18.66	18.66	2.890e+000	3.060e+000	1.700e-001
Fluorapatite	-0.00	-25.16	-25.16	1.700e-002	1.580e-002	-1.200e-003
Gypsum	0.00	-4.53	-4.53	1.300e-003	1.315e-001	1.302e-001
Halite	-5.38	-3.81	1.56	9.000e-004		-9.000e-004
Illite	-0.40	8.48	8.88	4.100e+000		-4.100e+000
K-Feldspar	-0.00	-0.38	-0.38	7.800e+000	1.026e+001	2.461e+000
Kaolinite	0.00	6.72	6.72	0.000e+000	3.597e+000	3.597e+000
Niter	-6.58	-6.81	-0.22	1.000e-003		-1.000e-003
O2(g)	-0.70	82.40	83.10	1.000e+000	3.618e-001	-6.382e-001
PuO2	0.00	-25.93	-25.93	8.760e-009	8.760e-009	-2.901e-013
Pyrite	-242.00	-325.69	-83.69	1.700e-001		-1.700e-001
Quartz	0.00	-4.03	-4.03	1.065e+002	1.059e+002	-5.783e-001
Tb2O3	-7.09	40.01	47.10	3.000e-002		-3.000e-002
TcO2:2H2O(am)	-40.01	-77.23	-37.22	5.720e-008		-5.720e-008
Yb2O3	-9.39	38.41	47.80	9.400e-003		-9.400e-003
Zincite	0.00	11.20	11.20			
ZnS	is reactant		5.000e-002	4.988e-002	-1.208e-004	

------------------Solution composition------------------------------

Elements	Molality	Moles
Al	5.292e-008	4.972e-008
As	1.277e-003	1.200e-003
B	2.460e-001	2.311e-001
Ba	2.047e-008	1.923e-008
C	6.685e-002	6.281e-002
Ca	1.094e-002	1.028e-002
Cl	1.183e-003	1.111e-003
F	1.277e-003	1.200e-003
Fe	4.660e-007	4.378e-007
I	1.010e-006	9.490e-007
K	3.562e-004	3.346e-004
Mg	9.261e-004	8.701e-004
Mn	6.061e-013	5.694e-013
N	1.294e-003	1.216e-003
Na	3.625e-001	3.406e-001
P	3.832e-003	3.600e-003
Pu	3.088e-013	2.901e-013
S	2.235e-001	2.100e-001
Se	1.916e-004	1.800e-004
Si	1.066e-004	1.002e-004
Tb	6.386e-002	6.000e-002
Tc	6.088e-008	5.720e-008
U	3.625e-006	3.406e-006
V	7.451e-003	7.000e-003
Yb	2.001e-002	1.880e-002
Zn	1.286e-004	1.208e-004

----------Description of solution----------

```
                                    pH  =   8.032  Charge balance
                                    pe  =  12.571  Adjusted to
redox equilibrium
                      Activity of water  =   0.986
                         Ionic strength  =  5.454e-001
                      Mass of water (kg)  =  9.395e-001
                Total alkalinity (eq/kg)  =  1.935e-001
                      Total CO2 (mol/kg)  =  6.685e-002
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  =  3.502e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                                Iterations  =  29
                                   Total H  = 1.049903e+002
                                   Total O  = 5.392986e+001
```

----------Distribution of species----------

Species	Molality	Log Activity	Molality	Log Activity	Log Gamma
OH-	1.555e-006	1.023e-006	-5.808	-5.990	-0.182
H+	1.158e-008	9.281e-009	-7.936	-8.032	-0.096
H2O	5.553e+001	9.856e-001	-0.006	-0.006	0.000
Al	5.292e-008				
AlO2-	5.062e-008	3.429e-008	-7.296	-7.465	-0.169
NaAlO2	1.363e-009	1.363e-009	-8.866	-8.866	0.000
HAlO2	9.289e-010	9.289e-010	-9.032	-9.032	0.000
Al(OH)2+	8.747e-012	5.924e-012	-11.058	-11.227	-0.169
AlOH+2	1.203e-013	2.403e-014	-12.920	-13.619	-0.700
Al(SO4)2-	1.404e-015	9.508e-016	-14.853	-15.022	-0.169
AlSO4+	7.428e-016	5.031e-016	-15.129	-15.298	-0.169
Al+3	2.239e-016	2.019e-017	-15.650	-16.695	-1.045
AlHPO4+	1.197e-016	8.109e-017	-15.922	-16.091	-0.169
Al2(OH)2+4	3.447e-023	9.386e-026	-22.462	-25.028	-2.565
AlF+2	4.639e-024	9.267e-025	-23.334	-24.033	-0.700
AlH2PO4+2	1.889e-028	3.772e-029	-27.724	-28.423	-0.700
Al3(OH)4+5	9.130e-029	1.380e-032	-28.040	-31.860	-3.821
AlF2+	2.499e-033	1.693e-033	-32.602	-32.771	-0.169
AlF3	0.000e+000	0.000e+000	-43.010	-43.010	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-51.392	-58.901	-7.510
AlF4-	0.000e+000	0.000e+000	-54.779	-54.948	-0.169
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-185.600	-185.600	0.000
As(3)	0.000e+000				
HAsO2	0.000e+000	0.000e+000	-57.042	-57.042	0.000
As(OH)3	0.000e+000	0.000e+000	-57.106	-57.106	0.000
H2AsO3-	0.000e+000	0.000e+000	-58.118	-58.288	-0.169
AsO2-	0.000e+000	0.000e+000	-58.132	-58.301	-0.169

AsO2OH-2	0.000e+000	0.000e+000	-60.521	-61.265	-0.744
HAsS2	0.000e+000	0.000e+000	-333.373	-333.373	0.000
As(5)	1.277e-003				
AsO3F-2	1.275e-003	2.299e-004	-2.895	-3.639	-0.744
HAsO3F-	2.339e-006	1.584e-006	-5.631	-5.800	-0.169
HAsO4-2	2.785e-028	5.022e-029	-27.555	-28.299	-0.744
H2AsO4-	4.146e-030	2.808e-030	-29.382	-29.552	-0.169
AsO4-3	6.989e-031	1.388e-032	-30.156	-31.858	-1.702
H3AsO4	4.591e-036	4.591e-036	-35.338	-35.338	0.000
B(-5)	0.000e+000				
BH4-	0.000e+000	0.000e+000	-222.362	-222.531	-0.169
B(3)	2.460e-001				
B(OH)3	2.201e-001	2.201e-001	-0.657	-0.657	0.000
BO2-	1.904e-002	1.290e-002	-1.720	-1.889	-0.169
NaB(OH)4	5.169e-003	5.169e-003	-2.287	-2.287	0.000
CaB(OH)4+	1.624e-003	1.100e-003	-2.789	-2.959	-0.169
MgB(OH)4+	1.288e-004	8.725e-005	-3.890	-4.059	-0.169
BaB(OH)4+	2.178e-009	1.475e-009	-8.662	-8.831	-0.169
B2O(OH)5-	1.591e-012	1.077e-012	-11.798	-11.968	-0.169
BF2(OH)2-	2.669e-031	1.808e-031	-30.574	-30.743	-0.169
BF3OH-	0.000e+000	0.000e+000	-46.308	-46.477	-0.169
BF4-	0.000e+000	0.000e+000	-63.851	-64.020	-0.169
Ba	2.047e-008				
Ba+2	1.825e-008	3.993e-009	-7.739	-8.399	-0.660
BaB(OH)4+	2.178e-009	1.475e-009	-8.662	-8.831	-0.169
BaNO3+	3.832e-011	2.596e-011	-10.417	-10.586	-0.169
BaCO3	4.646e-012	4.646e-012	-11.333	-11.333	0.000
BaCl+	1.454e-012	9.849e-013	-11.837	-12.007	-0.169
BaOH+	2.122e-014	1.437e-014	-13.673	-13.843	-0.169
BaF+	C(-2)	0.000e+000			
C2H4	0.000e+000	0.000e+000	-266.310	-266.310	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-238.631	-238.631	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-148.248	-148.248	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-51.206	-51.206	0.000
C(4)	6.685e-002				
TbCO3+	2.687e-002	1.820e-002	-1.571	-1.740	-0.169
YbCO3+	9.875e-003	6.688e-003	-2.005	-2.175	-0.169
Tb(CO3)2-	9.715e-003	6.580e-003	-2.013	-2.182	-0.169
Yb(CO3)2-	4.866e-003	3.296e-003	-2.313	-2.482	-0.169
HCO3-	7.357e-004	4.982e-004	-3.133	-3.303	-0.169
NaHCO3	1.485e-004	1.485e-004	-3.828	-3.828	0.000
CO3-2	1.192e-005	2.382e-006	-4.924	-5.623	-0.700
TbHCO3+2	1.097e-005	2.191e-006	-4.960	-5.659	-0.700
CaHCO3+	1.085e-005	7.345e-006	-4.965	-5.134	-0.169
CO2	9.594e-006	1.088e-005	-5.018	-4.963	0.055
CaCO3	6.867e-006	6.867e-006	-5.163	-5.163	0.000
UO2(CO3)3-4	3.426e-006	3.103e-009	-5.465	-8.508	-3.043
NaCO3-	2.564e-006	1.736e-006	-5.591	-5.760	-0.169

YbHCO3+2	2.413e-006	4.819e-007	-5.617	-6.317	-0.700
MgHCO3+	7.088e-007	4.800e-007	-6.149	-6.319	-0.169
ZnCO3	2.765e-007	2.765e-007	-6.558	-6.558	0.000
ZnHCO3+	2.621e-007	1.775e-007	-6.582	-6.751	-0.169
MgCO3	2.090e-007	2.090e-007	-6.680	-6.680	0.000
UO2(CO3)2-2	1.606e-007	2.895e-008	-6.794	-7.538	-0.744
(UO2)2CO3(OH)3-	1.589e-009	1.076e-009	-8.799	-8.968	-0.169
UO2CO3	6.320e-010	6.320e-010	-9.199	-9.199	0.000
BaCO3	4.646e-012	4.646e-012	-11.333	-11.333	0.000
(UO2)3(CO3)6-6	2.591e-013	3.456e-020	-12.587	-19.461	-6.875
PuO2(CO3)2-2	2.396e-013	4.320e-014	-12.621	-13.365	-0.744
FeCO3+	7.391e-015	5.006e-015	-14.131	-14.301	-0.169
MnCO3	4.895e-015	4.895e-015	-14.310	-14.310	0.000
MnHCO3+	3.288e-016	2.227e-016	-15.483	-15.652	-0.169
FeHCO3+	3.931e-019	2.663e-019	-18.405	-18.575	-0.169
FeCO3	1.377e-019	1.377e-019	-18.861	-18.861	0.000
(UO2)3(OH)5CO2+	3.324e-021	2.251e-021	-20.478	-20.648	-0.169
(UO2)3O(OH)2(HCO3)+	2.719e-021	1.842e-021	-20.566	-20.735	-0.169
UO2(CO3)3-5	9.236e-030	1.578e-034	-29.035	-33.802	-4.767
U(CO3)4-4	0.000e+000	0.000e+000	-45.777	-48.820	-3.043
(UO2)11(CO3)6(OH)12-2	0.000e+000	0.000e+000	-46.342	-47.086	-0.744
U(CO3)5-6	0.000e+000	0.000e+000	-48.651	-55.526	-6.875
SCN-	0.000e+000	0.000e+000	-214.854	-215.036	-0.182
UO2SCN+	0.000e+000	0.000e+000	-226.733	-226.902	-0.169
USCN+3	0.000e+000	0.000e+000	-272.031	-273.544	-1.513
Zn(SCN)2	0.000e+000	0.000e+000	-434.051	-434.051	0.000
UO2(SCN)2	0.000e+000	0.000e+000	-442.106	-442.106	0.000
U(SCN)2+2	0.000e+000	0.000e+000	-486.579	-487.279	-0.700
UO2(SCN)3-	0.000e+000	0.000e+000	-656.113	-656.282	-0.169
Zn(SCN)4-2	0.000e+000	0.000e+000	-863.011	-863.755	-0.744
Ca	1.094e-002				
Ca+2	4.868e-003	1.244e-003	-2.313	-2.905	-0.593
CaSO4	4.424e-003	4.424e-003	-2.354	-2.354	0.000
CaB(OH)4+	1.624e-003	1.100e-003	-2.789	-2.959	-0.169
CaHCO3+	1.085e-005	7.345e-006	-4.965	-5.134	-0.169
CaNO3+	7.534e-006	5.102e-006	-5.123	-5.292	-0.169
CaCO3	6.867e-006	6.867e-006	-5.163	-5.163	0.000
CaCl+	2.862e-007	1.939e-007	-6.543	-6.712	-0.169
CaHPO4	1.093e-007	1.093e-007	-6.961	-6.961	0.000
CaPO4-	4.349e-008	2.946e-008	-7.362	-7.531	-0.169
CaOH+	2.755e-008	1.866e-008	-7.560	-7.729	-0.169
CaCl2	1.676e-010	1.676e-010	-9.776	-9.776	0.000
CaP2O7-2	2.025e-013	3.650e-014	-12.694	-13.438	-0.744
CaH2PO4+	6.846e-017	4.637e-017	-16.165	-16.334	-0.169
CaF+	4.284e-017	2.902e-017	-16.368	-16.537	-0.169
Cl(-1)	1.183e-003				
Cl-	1.155e-003	7.352e-004	-2.937	-3.134	-0.196
NaCl	2.692e-005	2.692e-005	-4.570	-4.570	0.000
TbCl+2	5.515e-007	1.102e-007	-6.258	-6.958	-0.700
CaCl+	2.862e-007	1.939e-007	-6.543	-6.712	-0.169

YbCl+2	7.390e-008	1.476e-008	-7.131	-7.831	-0.700
MgCl+	7.030e-008	4.761e-008	-7.153	-7.322	-0.169
Zn(OH)Cl	3.100e-008	3.100e-008	-7.509	-7.509	0.000
ZnCl+	2.521e-008	1.707e-008	-7.598	-7.768	-0.169
KCl	4.725e-009	4.725e-009	-8.326	-8.326	0.000
CaCl2	1.676e-010	1.676e-010	-9.776	-9.776	0.000
TbCl2+	6.547e-011	4.434e-011	-10.184	-10.353	-0.169
ZnCl2	1.466e-011	1.466e-011	-10.834	-10.834	0.000
YbCl2+	6.349e-012	4.300e-012	-11.197	-11.367	-0.169
HCl	1.533e-012	1.533e-012	-11.815	-11.815	0.000
BaCl+	1.454e-012	9.849e-013	-11.837	-12.007	-0.169
TbCl3	1.278e-014	1.278e-014	-13.893	-13.893	0.000
ZnCl3-	8.791e-015	5.954e-015	-14.056	-14.225	-0.169
YbCl3	1.013e-015	1.013e-015	-14.995	-14.995	0.000
ZnCl4-2	1.840e-016	3.318e-017	-15.735	-16.479	-0.744
MnCl+	1.357e-016	9.191e-017	-15.867	-16.037	-0.169
UO2Cl+	8.541e-017	5.784e-017	-16.069	-16.238	-0.169
TbCl4-	5.096e-018	3.452e-018	-17.293	-17.462	-0.169
YbCl4-	4.071e-019	2.758e-019	-18.390	-18.559	-0.169
PuO2Cl+	5.590e-021	3.786e-021	-20.253	-20.422	-0.169
UO2Cl2	2.177e-021	2.177e-021	-20.662	-20.662	0.000
FeCl+	8.053e-022	5.454e-022	-21.094	-21.263	-0.169
FeCl+2	2.232e-022	4.459e-023	-21.651	-22.351	-0.700
FeCl2+	3.918e-023	2.654e-023	-22.407	-22.576	-0.169
MnCl3-	1.602e-023	1.085e-023	-22.795	-22.964	-0.169
FeCl2	2.152e-027	2.152e-027	-26.667	-26.667	0.000
FeCl4-	2.546e-032	1.725e-032	-31.594	-31.763	-0.169
FeCl4-2	1.864e-032	3.361e-033	-31.730	-32.474	-0.744
UCl+3	0.000e+000	0.000e+000	-61.390	-62.902	-1.513
Cl(1)	1.658e-020				
ClO-	1.344e-020	9.105e-021	-19.871	-20.041	-0.169
HClO	3.134e-021	3.134e-021	-20.504	-20.504	0.000
Cl(3)	2.122e-030				
ClO2-	2.122e-030	1.437e-030	-29.673	-29.842	-0.169
HClO2	1.972e-035	1.972e-035	-34.705	-34.705	0.000
Cl(5)	2.454e-026				
ClO3-	2.454e-026	1.615e-026	-25.610	-25.792	-0.182
UO2ClO3+	4.041e-039	2.737e-039	-38.394	-38.563	-0.169
Cl(7)	1.376e-026				
ClO4-	1.376e-026	9.053e-027	-25.861	-26.043	-0.182
ZnClO4+	3.495e-030	2.367e-030	-29.457	-29.626	-0.169
F	1.277e-003				
AsO3F-2	1.275e-003	2.299e-004	-2.895	-3.639	-0.744
HAsO3F-	2.339e-006	1.584e-006	-5.631	-5.800	-0.169
TbF+2	9.274e-014	1.852e-014	-13.033	-13.732	-0.700
YbF+2	2.064e-014	4.123e-015	-13.685	-14.385	-0.700
F-	6.974e-015	4.589e-015	-14.157	-14.338	-0.182
NaF	1.023e-016	1.023e-016	-15.990	-15.990	0.000
CaF+	4.284e-017	2.902e-017	-16.368	-16.537	-0.169
MgF+	1.356e-017	9.186e-018	-16.868	-17.037	-0.169
ZnF+	1.323e-018	8.959e-019	-17.878	-18.048	-0.169

HF	6.538e-020	6.538e-020	-19.185	-19.185	0.000
PO3F-2	6.062e-022	1.093e-022	-21.217	-21.961	-0.744
UO2F+	4.224e-023	2.861e-023	-22.374	-22.544	-0.169
BaF+	1.864e-023	1.262e-023	-22.730	-22.899	-0.169
AlF+2	4.639e-024	9.267e-025	-23.334	-24.033	-0.700
VO2F	1.523e-024	1.523e-024	-23.817	-23.817	0.000
TbF2+	4.047e-025	2.741e-025	-24.393	-24.562	-0.169
YbF2+	1.073e-025	7.268e-026	-24.969	-25.139	-0.169
PuO2F+	2.660e-026	1.802e-026	-25.575	-25.744	-0.169
HPO3F-	1.883e-026	1.276e-026	-25.725	-25.894	-0.169
MnF+	1.071e-026	7.251e-027	-25.970	-26.140	-0.169
FeF+2	1.254e-028	2.504e-029	-27.902	-28.601	-0.700
BF2(OH)2-	2.669e-031	1.808e-031	-30.574	-30.743	-0.169
FeF+	1.580e-031	1.070e-031	-30.801	-30.970	-0.169
AlF2+	2.499e-033	1.693e-033	-32.602	-32.771	-0.169
H2PO3F	7.573e-034	7.573e-034	-33.121	-33.121	0.000
UO2F2	3.939e-034	3.939e-034	-33.405	-33.405	0.000
HF2-	1.073e-034	7.267e-035	-33.969	-34.139	-0.169
VOF+	1.935e-035	1.310e-035	-34.713	-34.883	-0.169
PuO2F2	1.634e-035	1.634e-035	-34.787	-34.787	0.000
VO2F2-	2.976e-036	2.015e-036	-35.526	-35.696	-0.169
TbF3	4.609e-037	4.609e-037	-36.336	-36.336	0.000
YbF3	1.656e-037	1.656e-037	-36.781	-36.781	0.000
H2F2	1.063e-038	1.063e-038	-37.973	-37.973	0.000
FeF2+	2.746e-039	1.860e-039	-38.561	-38.731	-0.169
AlF3	0.000e+000	0.000e+000	-43.010	-43.010	0.000
PuF+3	0.000e+000	0.000e+000	-43.844	-45.356	-1.513
PuO2F3-	0.000e+000	0.000e+000	-43.990	-44.160	-0.169
UO2F3-	0.000e+000	0.000e+000	-45.307	-45.476	-0.169
BF3OH-	0.000e+000	0.000e+000	-46.308	-46.477	-0.169
VOF2	0.000e+000	0.000e+000	-46.441	-46.441	0.000
TbF4-	0.000e+000	0.000e+000	-48.430	-48.599	-0.169
YbF4-	0.000e+000	0.000e+000	-48.777	-48.946	-0.169
PuF2+2	0.000e+000	0.000e+000	-52.055	-52.755	-0.700
AlF4-	0.000e+000	0.000e+000	-54.779	-54.948	-0.169
PuO2F4-2	0.000e+000	0.000e+000	-54.880	-55.624	-0.744
UO2F4-2	0.000e+000	0.000e+000	-58.295	-59.039	-0.744
BF4-	0.000e+000	0.000e+000	-63.851	-64.020	-0.169
UF+3	0.000e+000	0.000e+000	-65.050	-66.563	-1.513
UF2+2	0.000e+000	0.000e+000	-73.276	-73.975	-0.700
PuF3+	0.000e+000	0.000e+000	-77.024	-77.193	-0.169
UF3+	0.000e+000	0.000e+000	-82.793	-82.962	-0.169
PuF4	0.000e+000	0.000e+000	-92.631	-92.631	0.000
UF4	0.000e+000	0.000e+000	-93.357	-93.357	0.000
SiF6-2	0.000e+000	0.000e+000	-95.044	-95.788	-0.744
UF5-	0.000e+000	0.000e+000	-106.198	-106.367	-0.169
UF6-2	0.000e+000	0.000e+000	-117.931	-118.675	-0.744
Fe(2)	8.498e-018				
Fe+2	3.985e-018	1.018e-018	-17.400	-17.992	-0.593
FeSO4	3.929e-018	3.929e-018	-17.406	-17.406	0.000
FeHCO3+	3.931e-019	2.663e-019	-18.405	-18.575	-0.169

FeCO3	1.377e-019	1.377e-019	-18.861	-18.861	0.000
FeOH+	5.049e-020	3.420e-020	-19.297	-19.466	-0.169
FePO4-	1.051e-021	7.116e-022	-20.979	-21.148	-0.169
FeCl+	8.053e-022	5.454e-022	-21.094	-21.263	-0.169
FeHPO4	6.481e-022	6.481e-022	-21.188	-21.188	0.000
Fe(OH)2	2.885e-023	2.885e-023	-22.540	-22.540	0.000
Fe(OH)3-	1.801e-025	1.219e-025	-24.745	-24.914	-0.169
FeCl2	2.152e-027	2.152e-027	-26.667	-26.667	0.000
FeH2PO4+	1.118e-030	7.572e-031	-29.952	-30.121	-0.169
FeF+	1.580e-031	1.070e-031	-30.801	-30.970	-0.169
Fe(OH)4-2	7.183e-032	1.295e-032	-31.144	-31.888	-0.744
FeCl4-2	1.864e-032	3.361e-033	-31.730	-32.474	-0.744
Fe(3)	4.660e-007				
Fe(OH)3	4.359e-007	4.359e-007	-6.361	-6.361	0.000
Fe(OH)4-	1.717e-008	1.163e-008	-7.765	-7.935	-0.169
Fe(OH)2+	1.296e-008	8.775e-009	-7.888	-8.057	-0.169
FeOH+2	1.249e-012	2.495e-013	-11.903	-12.603	-0.700
FeCO3+	7.391e-015	5.006e-015	-14.131	-14.301	-0.169
FeHPO4+	1.300e-015	8.806e-016	-14.886	-15.055	-0.169
Fe+3	4.034e-018	3.639e-019	-17.394	-18.439	-1.045
FeSO4+	1.266e-018	8.573e-019	-17.898	-18.067	-0.169
Fe(SO4)2-	5.210e-019	3.528e-019	-18.283	-18.452	-0.169
FeNO3+2	1.491e-020	2.978e-021	-19.827	-20.526	-0.700
Fe2(OH)2+4	6.156e-022	1.676e-024	-21.211	-23.776	-2.565
FeCl+2	2.232e-022	4.459e-023	-21.651	-22.351	-0.700
FeCl2+	3.918e-023	2.654e-023	-22.407	-22.576	-0.169
Fe3(OH)4+5	2.033e-026	3.073e-030	-25.692	-29.512	-3.821
FeF+2	1.254e-028	2.504e-029	-27.902	-28.601	-0.700
FeH2PO4+2	3.999e-029	7.987e-030	-28.398	-29.098	-0.700
FeNO2+2	7.703e-032	1.539e-032	-31.113	-31.813	-0.700
FeCl4-	2.546e-032	1.725e-032	-31.594	-31.763	-0.169
FeF2+	2.746e-039	1.860e-039	-38.561	-38.731	-0.169
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-44.363	-44.308	0.055
I(-03)	0.000e+000				
I3-	0.000e+000	0.000e+000	-48.263	-48.432	-0.169
I(-1)	5.662e-019				
I-	5.639e-019	3.590e-019	-18.249	-18.445	-0.196
NaI	2.251e-021	2.251e-021	-20.648	-20.648	0.000
KI	1.776e-024	1.776e-024	-23.751	-23.751	0.000
ZnI+	7.104e-027	4.812e-027	-26.148	-26.318	-0.169
ZnI2	0.000e+000	0.000e+000	-43.593	-43.593	0.000
ZnI3-	0.000e+000	0.000e+000	-62.030	-62.200	-0.169
UI+3	0.000e+000	0.000e+000	-77.203	-78.716	-1.513
ZnI4-2	0.000e+000	0.000e+000	-80.500	-81.244	-0.744
I(1)	1.033e-021				
IO-	1.033e-021	6.996e-022	-20.986	-21.155	-0.169
I(5)	1.010e-006				
IO3-	1.010e-006	6.841e-007	-5.996	-6.165	-0.169
HIO3	1.969e-014	1.969e-014	-13.706	-13.706	0.000
UO2IO3+	2.825e-018	1.913e-018	-17.549	-17.718	-0.169

UO2(IO3)2	2.457e-023	2.457e-023	-22.610	-22.610	0.000
I(7)	3.191e-019				
IO4-	3.191e-019	2.100e-019	-18.496	-18.678	-0.182
K	3.562e-004				
K+	3.007e-004	1.914e-004	-3.522	-3.718	-0.196
KSO4-	5.553e-005	3.761e-005	-4.255	-4.425	-0.169
KCl	4.725e-009	4.725e-009	-8.326	-8.326	0.000
KHPO4-	2.722e-010	1.844e-010	-9.565	-9.734	-0.169
KOH	7.047e-011	7.047e-011	-10.152	-10.152	0.000
KHSO4	3.080e-013	3.080e-013	-12.511	-12.511	0.000
KP2O7-3	1.065e-017	2.116e-019	-16.973	-18.675	-1.702
KI	1.776e-024	1.776e-024	-23.751	-23.751	0.000
Mg	9.261e-004				
MgSO4	5.393e-004	5.393e-004	-3.268	-3.268	0.000
Mg+2	2.570e-004	8.295e-005	-3.590	-4.081	-0.491
MgB(OH)4+	1.288e-004	8.725e-005	-3.890	-4.059	-0.169
MgHCO3+	7.088e-007	4.800e-007	-6.149	-6.319	-0.169
MgCO3	2.090e-007	2.090e-007	-6.680	-6.680	0.000
MgCl+	7.030e-008	4.761e-008	-7.153	-7.322	-0.169
MgHPO4	1.078e-008	1.078e-008	-7.967	-7.967	0.000
MgPO4-	3.903e-009	2.643e-009	-8.409	-8.578	-0.169
MgP2O7-2	3.997e-014	7.207e-015	-13.398	-14.142	-0.744
MgF+	1.356e-017	9.186e-018	-16.868	-17.037	-0.169
MgH2PO4+	8.307e-018	5.626e-018	-17.081	-17.250	-0.169
Mg4(OH)4+4	3.934e-022	1.071e-024	-21.405	-23.970	-2.565
Mn(2)	5.887e-013				
MnSO4	3.527e-013	3.527e-013	-12.453	-12.453	0.000
Mn+2	2.297e-013	5.871e-014	-12.639	-13.231	-0.593
MnCO3	4.895e-015	4.895e-015	-14.310	-14.310	0.000
MnSeO4	5.457e-016	5.457e-016	-15.263	-15.263	0.000
MnHCO3+	3.288e-016	2.227e-016	-15.483	-15.652	-0.169
MnOH+	2.366e-016	1.603e-016	-15.626	-15.795	-0.169
MnCl+	1.357e-016	9.191e-017	-15.867	-16.037	-0.169
MnNO3+	1.124e-016	7.615e-017	-15.949	-16.118	-0.169
MnHPO4	3.568e-017	3.568e-017	-16.448	-16.448	0.000
MnPO4-	1.102e-017	7.465e-018	-16.958	-17.127	-0.169
Mn(NO3)2	1.565e-019	1.565e-019	-18.805	-18.805	0.000
MnH2PO4+	4.621e-020	3.130e-020	-19.335	-19.505	-0.169
Mn(OH)2	4.178e-020	4.178e-020	-19.379	-19.379	0.000
MnCl3-	1.602e-023	1.085e-023	-22.795	-22.964	-0.169
Mn(OH)3-	6.144e-024	4.161e-024	-23.212	-23.381	-0.169
MnF+	1.071e-026	7.251e-027	-25.970	-26.140	-0.169
Mn2(OH)3+	7.673e-027	5.197e-027	-26.115	-26.284	-0.169
Mn2OH+3	3.284e-028	1.008e-029	-27.484	-28.996	-1.513
Mn(OH)4-2	2.076e-029	3.742e-030	-28.683	-29.427	-0.744
Mn(3)	1.901e-025				
Mn+3	1.901e-025	5.837e-027	-24.721	-26.234	-1.513
Mn(6)	3.850e-017				
MnO4-2	3.850e-017	6.942e-018	-16.414	-17.158	-0.744
Mn(7)	1.732e-014				
MnO4-	1.732e-014	1.140e-014	-13.761	-13.943	-0.182
N(-03)	0.000e+000				

N3-	0.000e+000	0.000e+000	-100.039	-100.208	-0.169
HN3	0.000e+000	0.000e+000	-103.538	-103.538	0.000
ZnN3+	0.000e+000	0.000e+000	-104.456	-104.625	-0.169
UO2N3+	0.000e+000	0.000e+000	-110.736	-110.905	-0.169
Zn(N3)2	0.000e+000	0.000e+000	-204.080	-204.080	0.000
UO2(N3)2	0.000e+000	0.000e+000	-209.363	-209.363	0.000
UO2(N3)3-	0.000e+000	0.000e+000	-307.991	-308.160	-0.169
UO2(N3)4-2	0.000e+000	0.000e+000	-408.445	-409.189	-0.744
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-64.589	-64.801	-0.213
NH3	0.000e+000	0.000e+000	-66.009	-66.009	0.000
Zn(NH3)+2	0.000e+000	0.000e+000	-68.116	-68.816	-0.700
NH4SO4-	0.000e+000	0.000e+000	-74.546	-74.715	-0.169
Zn(NH3)2+2	0.000e+000	0.000e+000	-131.919	-132.619	-0.700
Zn(NH3)3+2	0.000e+000	0.000e+000	-195.722	-196.421	-0.700
SCN-	0.000e+000	0.000e+000	-214.854	-215.036	-0.182
UO2SCN+	0.000e+000	0.000e+000	-226.733	-226.902	-0.169
Zn(NH3)4+2	0.000e+000	0.000e+000	-259.798	-260.498	-0.700
USCN+3	0.000e+000	0.000e+000	-272.031	-273.544	-1.513
Zn(SCN)2	0.000e+000	0.000e+000	-434.051	-434.051	0.000
UO2(SCN)2	0.000e+000	0.000e+000	-442.106	-442.106	0.000
U(SCN)2+2	0.000e+000	0.000e+000	-486.579	-487.279	-0.700
UO2(SCN)3-	0.000e+000	0.000e+000	-656.113	-656.282	-0.169
Zn(SCN)4-2	0.000e+000	0.000e+000	-863.011	-863.755	-0.744
N(-5)	0.000e+000				
HCN	0.000e+000	0.000e+000	-122.324	-122.324	0.000
CN-	0.000e+000	0.000e+000	-123.354	-123.550	-0.196
Zn(CN)4-2	0.000e+000	0.000e+000	-481.541	-482.285	-0.744
N(0)	2.354e-021				
N2	1.177e-021	1.177e-021	-20.929	-20.929	0.000
N(3)	4.702e-017				
NO2-	4.702e-017	2.993e-017	-16.328	-16.524	-0.196
HNO2	4.741e-022	4.741e-022	-21.324	-21.324	0.000
FeNO2+2	7.703e-032	1.539e-032	-31.113	-31.813	-0.700
N(5)	1.294e-003				
NO3-	1.285e-003	8.183e-004	-2.891	-3.087	-0.196
CaNO3+	7.534e-006	5.102e-006	-5.123	-5.292	-0.169
TbNO3+2	1.158e-006	2.312e-007	-5.936	-6.636	-0.700
YbNO3+2	9.308e-008	1.859e-008	-7.031	-7.731	-0.700
BaNO3+	3.832e-011	2.596e-011	-10.417	-10.586	-0.169
HNO3	3.972e-013	3.972e-013	-12.401	-12.401	0.000
UO2NO3+	1.219e-016	8.256e-017	-15.914	-16.083	-0.169
MnNO3+	1.124e-016	7.615e-017	-15.949	-16.118	-0.169
Mn(NO3)2	1.565e-019	1.565e-019	-18.805	-18.805	0.000
FeNO3+2	1.491e-020	2.978e-021	-19.827	-20.526	-0.700
UNO3+3	0.000e+000	0.000e+000	-61.610	-63.123	-1.513
U(NO3)2+2	0.000e+000	0.000e+000	-64.700	-65.399	-0.700
Na	3.625e-001				
Na+	3.076e-001	2.084e-001	-0.512	-0.681	-0.169
NaSO4-	4.948e-002	3.351e-002	-1.306	-1.475	-0.169
NaB(OH)4	5.169e-003	5.169e-003	-2.287	-2.287	0.000
NaHCO3	1.485e-004	1.485e-004	-3.828	-3.828	0.000

NaCl	2.692e-005	2.692e-005	-4.570	-4.570	0.000
NaHSiO3	1.117e-005	1.117e-005	-4.952	-4.952	0.000
NaCO3-	2.564e-006	1.736e-006	-5.591	-5.760	-0.169
NaHPO4-	4.091e-007	2.771e-007	-6.388	-6.557	-0.169
NaOH	3.678e-008	3.678e-008	-7.434	-7.434	0.000
NaAlO2	1.363e-009	1.363e-009	-8.866	-8.866	0.000
Na2P2O7-2	1.734e-014	3.127e-015	-13.761	-14.505	-0.744
NaP2O7-3	9.511e-015	1.889e-016	-14.022	-15.724	-1.702
NaHP2O7-2	1.968e-015	3.548e-016	-14.706	-15.450	-0.744
NaF	1.023e-016	1.023e-016	-15.990	-15.990	0.000
NaI	2.251e-021	2.251e-021	-20.648	-20.648	0.000
O(0)	4.507e-004				
O2	2.254e-004	2.556e-004	-3.647	-3.592	0.055
UO2S2O3	0.000e+000	0.000e+000	-156.680	-156.680	0.000
S3O6-2	0.000e+000	0.000e+000	-175.021	-175.765	-0.744
S2-2	0.000e+000	0.000e+000	-249.276	-250.020	-0.744
S4O6-2	0.000e+000	0.000e+000	-266.022	-266.766	-0.744
S3-2	0.000e+000	0.000e+000	-353.700	-354.444	-0.744
S5O6-2	0.000e+000	0.000e+000	-385.902	-386.646	-0.744
S4-2	0.000e+000	0.000e+000	-458.351	-459.095	-0.744
S5-2	0.000e+000	0.000e+000	-563.218	-563.962	-0.744
P(-3)	0.000e+000				
PH4+	0.000e+000	0.000e+000	-236.280	-236.450	-0.169
P(5)	3.832e-003				
TbPO4	1.700e-003	1.700e-003	-2.770	-2.770	0.000
YbPO4	8.516e-004	8.516e-004	-3.070	-3.070	0.000
Yb(PO4)2-3	3.519e-004	6.990e-006	-3.454	-5.156	-1.702
Tb(PO4)2-3	2.797e-004	5.555e-006	-3.553	-5.255	-1.702
TbHPO4+	1.228e-005	8.315e-006	-4.911	-5.080	-0.169
YbHPO4+	3.082e-006	2.088e-006	-5.511	-5.680	-0.169
HPO4-2	8.866e-007	1.599e-007	-6.052	-6.796	-0.744
NaHPO4-	4.091e-007	2.771e-007	-6.388	-6.557	-0.169
CaHPO4	1.093e-007	1.093e-007	-6.961	-6.961	0.000
CaPO4-	4.349e-008	2.946e-008	-7.362	-7.531	-0.169
H2PO4-	3.705e-008	2.509e-008	-7.431	-7.600	-0.169
ZnPO4-	1.755e-008	1.188e-008	-7.756	-7.925	-0.169
Tb(HPO4)2-	1.559e-008	1.056e-008	-7.807	-7.976	-0.169
MgHPO4	1.078e-008	1.078e-008	-7.967	-7.967	0.000
Yb(HPO4)2-	7.809e-009	5.289e-009	-8.107	-8.277	-0.169
ZnHPO4	4.021e-009	4.021e-009	-8.396	-8.396	0.000
MgPO4-	3.903e-009	2.643e-009	-8.409	-8.578	-0.169
TbH2PO4+2	1.628e-009	3.252e-010	-8.788	-9.488	-0.700
PO4-3	3.930e-010	7.807e-012	-9.406	-11.108	-1.702
YbH2PO4+2	3.591e-010	7.173e-011	-9.445	-10.144	-0.700
KHPO4-	2.722e-010	1.844e-010	-9.565	-9.734	-0.169
UO2PO4-	1.616e-010	1.095e-010	-9.792	-9.961	-0.169
UO2HPO4	2.327e-012	2.327e-012	-11.633	-11.633	0.000
CaP2O7-2	2.025e-013	3.650e-014	-12.694	-13.438	-0.744
MgP2O7-2	3.997e-014	7.207e-015	-13.398	-14.142	-0.744
H3PO4	3.588e-014	3.588e-014	-13.445	-13.445	0.000
VO2HPO4-	2.366e-014	1.602e-014	-13.626	-13.795	-0.169

Na2P2O7-2	1.734e-014	3.127e-015	-13.761	-14.505	-0.744
NaP2O7-3	9.511e-015	1.889e-016	-14.022	-15.724	-1.702
P2O7-4	5.558e-015	5.033e-018	-14.255	-17.298	-3.043
HP2O7-3	3.839e-015	7.626e-017	-14.416	-16.118	-1.702
NaHP2O7-2	1.968e-015	3.548e-016	-14.706	-15.450	-0.744
FeHPO4+	1.300e-015	8.806e-016	-14.886	-15.055	-0.169
AlHPO4+	1.197e-016	8.109e-017	-15.922	-16.091	-0.169
VO2(HPO4)2-3	7.593e-017	1.508e-018	-16.120	-17.822	-1.702
CaH2PO4+	6.846e-017	4.637e-017	-16.165	-16.334	-0.169
UO2H2PO4+	5.443e-017	3.686e-017	-16.264	-16.433	-0.169
MnHPO4	3.568e-017	3.568e-017	-16.448	-16.448	0.000
H2P2O7-2	1.624e-017	2.927e-018	-16.790	-17.534	-0.744
MnPO4-	1.102e-017	7.465e-018	-16.958	-17.127	-0.169
KP2O7-3	1.065e-017	2.116e-019	-16.973	-18.675	-1.702
MgH2PO4+	8.307e-018	5.626e-018	-17.081	-17.250	-0.169
ZnH2PO4+	8.150e-020	5.520e-020	-19.089	-19.258	-0.169
MnH2PO4+	4.621e-020	3.130e-020	-19.335	-19.505	-0.169
Pu(HPO4)4-4	5.761e-021	5.216e-024	-20.240	-23.283	-3.043
PuO2H2PO4+	3.108e-021	2.105e-021	-20.507	-20.677	-0.169
FePO4-	1.051e-021	7.116e-022	-20.979	-21.148	-0.169
FeHPO4	6.481e-022	6.481e-022	-21.188	-21.188	0.000
UO2(H2PO4)2	6.453e-022	6.453e-022	-21.190	-21.190	0.000
PO3F-2	6.062e-022	1.093e-022	-21.217	-21.961	-0.744
H3P2O7-	9.220e-024	6.245e-024	-23.035	-23.204	-0.169
UO2H3PO4+2	7.477e-025	1.493e-025	-24.126	-24.826	-0.700
Pu(HPO4)3-2	2.646e-026	4.771e-027	-25.577	-26.321	-0.744
HPO3F-	1.883e-026	1.276e-026	-25.725	-25.894	-0.169
VO2H2PO4	1.053e-026	1.053e-026	-25.978	-25.978	0.000
AlH2PO4+2	1.889e-028	3.772e-029	-27.724	-28.423	-0.700
UO2(H2PO4)(H3PO4)+	9.049e-029	6.129e-029	-28.043	-28.213	-0.169
FeH2PO4+2	3.999e-029	7.987e-030	-28.398	-29.098	-0.700
Pu(HPO4)2	6.557e-030	6.557e-030	-29.183	-29.183	0.000
H4P2O7	1.703e-030	1.703e-030	-29.769	-29.769	0.000
FeH2PO4+	1.118e-030	7.572e-031	-29.952	-30.121	-0.169
PuHPO4+2	2.969e-033	5.930e-034	-32.527	-33.227	-0.700
H2PO3F	7.573e-034	7.573e-034	-33.121	-33.121	0.000
PuH2PO4+2	3.473e-040	0.000e+000	-39.459	-40.159	-0.700
Pu(3)	1.752e-032				
Pu(SO4)2-	1.612e-032	1.092e-032	-31.793	-31.962	-0.169
PuSO4+	1.062e-033	7.192e-034	-32.974	-33.143	-0.169
Pu+3	2.872e-034	8.817e-036	-33.542	-35.055	-1.513
PuOH+2	5.023e-035	1.003e-035	-34.299	-34.999	-0.700
PuH2PO4+2	3.473e-040	0.000e+000	-39.459	-40.159	-0.700
Pu(4)	1.376e-017				
Pu(OH)4	1.375e-017	1.375e-017	-16.862	-16.862	0.000
Pu(HPO4)4-4	5.761e-021	5.216e-024	-20.240	-23.283	-3.043
Pu(OH)3+	3.020e-021	2.046e-021	-20.520	-20.689	-0.169
Pu(OH)2+2	8.892e-026	1.776e-026	-25.051	-25.751	-0.700
Pu(HPO4)3-2	2.646e-026	4.771e-027	-25.577	-26.321	-0.744
Pu(HPO4)2	6.557e-030	6.557e-030	-29.183	-29.183	0.000

PuOH+3	3.603e-031	1.106e-032	-30.443	-31.956	-1.513
Pu(SO4)2	3.730e-033	3.730e-033	-32.428	-32.428	0.000
PuHPO4+2	2.969e-033	5.930e-034	-32.527	-33.227	-0.700
PuSO4+2	2.597e-035	5.186e-036	-34.586	-35.285	-0.700
Pu+4	1.221e-037	3.325e-040	-36.913	-39.478	-2.565
PuF+3	0.000e+000	0.000e+000	-43.844	-45.356	-1.513
PuF2+2	0.000e+000	0.000e+000	-52.055	-52.755	-0.700
PuF3+	0.000e+000	0.000e+000	-77.024	-77.193	-0.169
PuF4	0.000e+000	0.000e+000	-92.631	-92.631	0.000
Pu(5)	6.586e-014				
PuO2+	6.484e-014	4.391e-014	-13.188	-13.357	-0.169
PuO2OH	1.021e-015	1.021e-015	-14.991	-14.991	0.000
Pu(6)	2.429e-013				
PuO2(CO3)2-2	2.396e-013	4.320e-014	-12.621	-13.365	-0.744
PuO2OH+	2.901e-015	1.965e-015	-14.537	-14.707	-0.169
PuO2SO4	3.719e-016	3.719e-016	-15.430	-15.430	0.000
PuO2+2	4.036e-017	8.061e-018	-16.394	-17.094	-0.700
PuO2Cl+	5.590e-021	3.786e-021	-20.253	-20.422	-0.169
PuO2H2PO4+	3.108e-021	2.105e-021	-20.507	-20.677	-0.169
PuO2F+	2.660e-026	1.802e-026	-25.575	-25.744	-0.169
(PuO2)2(OH)2+2	2.011e-026	4.017e-027	-25.697	-26.396	-0.700
(PuO2)3(OH)5+	2.296e-033	1.555e-033	-32.639	-32.808	-0.169
PuO2F2	1.634e-035	1.634e-035	-34.787	-34.787	0.000
PuO2F3-	0.000e+000	0.000e+000	-43.990	-44.160	-0.169
PuO2F4-2	0.000e+000	0.000e+000	-54.880	-55.624	-0.744
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-140.562	-140.744	-0.182
H2S	0.000e+000	0.000e+000	-141.767	-141.767	0.000
S-2	0.000e+000	0.000e+000	-144.977	-145.637	-0.660
SCN-	0.000e+000	0.000e+000	-214.854	-215.036	-0.182
UO2SCN+	0.000e+000	0.000e+000	-226.733	-226.902	-0.169
S2-2	0.000e+000	0.000e+000	-249.276	-250.020	-0.744
USCN+3	0.000e+000	0.000e+000	-272.031	-273.544	-1.513
HAsS2	0.000e+000	0.000e+000	-333.373	-333.373	0.000
S3-2	0.000e+000	0.000e+000	-353.700	-354.444	-0.744
Zn(SCN)2	0.000e+000	0.000e+000	-434.051	-434.051	0.000
UO2(SCN)2	0.000e+000	0.000e+000	-442.106	-442.106	0.000
S4-2	0.000e+000	0.000e+000	-458.351	-459.095	-0.744
U(SCN)2+2	0.000e+000	0.000e+000	-486.579	-487.279	-0.700
S5-2	0.000e+000	0.000e+000	-563.218	-563.962	-0.744
UO2(SCN)3-	0.000e+000	0.000e+000	-656.113	-656.282	-0.169
Zn(SCN)4-2	0.000e+000	0.000e+000	-863.011	-863.755	-0.744
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-144.831	-145.575	-0.744
HS2O3-	0.000e+000	0.000e+000	-152.424	-152.593	-0.169
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-134.136	-134.795	-0.660
S(4)	0.000e+000				
SO3-2	0.000e+000	0.000e+000	-45.736	-46.435	-0.700
HSO3-	0.000e+000	0.000e+000	-47.067	-47.236	-0.169
UO2SO3	0.000e+000	0.000e+000	-52.959	-52.959	0.000

H2SO3	0.000e+000	0.000e+000	-53.287	-53.287	0.000
SO2	0.000e+000	0.000e+000	-53.381	-53.381	0.000
UO2(SO3)2-2	0.000e+000	0.000e+000	-97.493	-98.237	-0.744
S2O5-2	0.000e+000	0.000e+000	-98.552	-99.296	-0.744
UO2S2O3	0.000e+000	0.000e+000	-156.680	-156.680	0.000
S3O6-2	0.000e+000	0.000e+000	-175.021	-175.765	-0.744
S4O6-2	0.000e+000	0.000e+000	-266.022	-266.766	-0.744
S5O6-2	0.000e+000	0.000e+000	-385.902	-386.646	-0.744
S(5)	0.000e+000				
S2O6-2	0.000e+000	0.000e+000	-68.114	-68.858	-0.744
S(6)	2.235e-001				
SO4-2	1.350e-001	2.435e-002	-0.870	-1.614	-0.744
NaSO4-	4.948e-002	3.351e-002	-1.306	-1.475	-0.169
TbSO4+	1.463e-002	9.907e-003	-1.835	-2.004	-0.169
Tb(SO4)2-	7.214e-003	4.886e-003	-2.142	-2.311	-0.169
CaSO4	4.424e-003	4.424e-003	-2.354	-2.354	0.000
YbSO4+	1.960e-003	1.328e-003	-2.708	-2.877	-0.169
Yb(SO4)2-	1.439e-003	9.744e-004	-2.842	-3.011	-0.169
MgSO4	5.393e-004	5.393e-004	-3.268	-3.268	0.000
ZnSO4	7.071e-005	7.071e-005	-4.151	-4.151	0.000
KSO4-	5.553e-005	3.761e-005	-4.255	-4.425	-0.169
HSO4-	3.370e-008	2.282e-008	-7.472	-7.642	-0.169
UO2(SO4)2-2	1.873e-012	3.377e-013	-11.727	-12.471	-0.744
UO2SO4	1.565e-012	1.565e-012	-11.805	-11.805	0.000
MnSO4	3.527e-013	3.527e-013	-12.453	-12.453	0.000
KHSO4	3.080e-013	3.080e-013	-12.511	-12.511	0.000
VO2SO4-	2.026e-013	1.372e-013	-12.693	-12.863	-0.169
Al(SO4)2-	1.404e-015	9.508e-016	-14.853	-15.022	-0.169
AlSO4+	7.428e-016	5.031e-016	-15.129	-15.298	-0.169
PuO2SO4	3.719e-016	3.719e-016	-15.430	-15.430	0.000
FeSO4	3.929e-018	3.929e-018	-17.406	-17.406	0.000
FeSO4+	1.266e-018	8.573e-019	-17.898	-18.067	-0.169
Fe(SO4)2-	5.210e-019	3.528e-019	-18.283	-18.452	-0.169
H2SO4	1.999e-019	1.999e-019	-18.699	-18.699	0.000
VOSO4	2.099e-024	2.099e-024	-23.678	-23.678	0.000
Pu(SO4)2-	1.612e-032	1.092e-032	-31.793	-31.962	-0.169
Pu(SO4)2	3.730e-033	3.730e-033	-32.428	-32.428	0.000
PuSO4+	1.062e-033	7.192e-034	-32.974	-33.143	-0.169
PuSO4+2	2.597e-035	5.186e-036	-34.586	-35.285	-0.700
VSO4+	0.000e+000	0.000e+000	-45.493	-45.662	-0.169
U(SO4)2	0.000e+000	0.000e+000	-54.339	-54.339	0.000
USO4+2	0.000e+000	0.000e+000	-55.866	-56.565	-0.700
NH4SO4-	0.000e+000	0.000e+000	-74.546	-74.715	-0.169
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-42.793	-43.537	-0.744
S(8)	2.927e-029				
HSO5-	2.927e-029	1.982e-029	-28.534	-28.703	-0.169
Se(-2)	0.000e+000				
HSe-	0.000e+000	0.000e+000	-95.931	-96.100	-0.169
H2Se	0.000e+000	0.000e+000	-100.311	-100.311	0.000
Se-2	0.000e+000	0.000e+000	-102.270	-103.014	-0.744

Se(4)	1.314e-016				
SeO3-2	1.251e-016	2.255e-017	-15.903	-16.647	-0.744
HSeO3-	6.352e-018	4.302e-018	-17.197	-17.366	-0.169
H2SeO3	1.517e-023	1.517e-023	-22.819	-22.819	0.000
Se(6)	1.916e-004				
SeO4-2	1.915e-004	3.453e-005	-3.718	-4.462	-0.744
ZnSeO4	7.393e-008	7.393e-008	-7.131	-7.131	0.000
HSeO4-	4.024e-011	2.726e-011	-10.395	-10.565	-0.169
MnSeO4	5.457e-016	5.457e-016	-15.263	-15.263	0.000
Si	1.066e-004				
SiO2	9.379e-005	9.379e-005	-4.028	-4.028	0.000
NaHSiO3	1.117e-005	1.117e-005	-4.952	-4.952	0.000
HSiO3-	1.680e-006	1.138e-006	-5.775	-5.944	-0.169
H2SiO4-2	6.432e-011	1.160e-011	-10.192	-10.936	-0.744
H6(H2SiO4)4-2	1.016e-013	1.833e-014	-12.993	-13.737	-0.744
H4(H2SiO4)4-4	1.177e-017	1.066e-020	-16.929	-19.972	-3.043
SiF6-2	0.000e+000	0.000e+000	-95.044	-95.788	-0.744
Tb(2)	0.000e+000				
Tb+2	0.000e+000	0.000e+000	-73.232	-73.932	-0.700
Tb(3)	6.386e-002				
TbCO3+	2.687e-002	1.820e-002	-1.571	-1.740	-0.169
TbSO4+	1.463e-002	9.907e-003	-1.835	-2.004	-0.169
Tb(CO3)2-	9.715e-003	6.580e-003	-2.013	-2.182	-0.169
Tb(SO4)2-	7.214e-003	4.886e-003	-2.142	-2.311	-0.169
Tb+3	2.685e-003	8.244e-005	-2.571	-4.084	-1.513
TbPO4	1.700e-003	1.700e-003	-2.770	-2.770	0.000
TbOH+2	6.497e-004	1.298e-004	-3.187	-3.887	-0.700
Tb(PO4)2-3	2.797e-004	5.555e-006	-3.553	-5.255	-1.702
TbO+	9.052e-005	6.131e-005	-4.043	-4.212	-0.169
TbHPO4+	1.228e-005	8.315e-006	-4.911	-5.080	-0.169
TbHCO3+2	1.097e-005	2.191e-006	-4.960	-5.659	-0.700
TbO2H	8.678e-006	8.678e-006	-5.062	-5.062	0.000
TbNO3+2	1.158e-006	2.312e-007	-5.936	-6.636	-0.700
TbO2-	9.493e-007	6.429e-007	-6.023	-6.192	-0.169
TbCl+2	5.515e-007	1.102e-007	-6.258	-6.958	-0.700
Tb(HPO4)2-	1.559e-008	1.056e-008	-7.807	-7.976	-0.169
TbH2PO4+2	1.628e-009	3.252e-010	-8.788	-9.488	-0.700
TbCl2+	6.547e-011	4.434e-011	-10.184	-10.353	-0.169
TbF+2	9.274e-014	1.852e-014	-13.033	-13.732	-0.700
TbCl3	1.278e-014	1.278e-014	-13.893	-13.893	0.000
TbCl4-	5.096e-018	3.452e-018	-17.293	-17.462	-0.169
TbF2+	4.047e-025	2.741e-025	-24.393	-24.562	-0.169
TbF3	4.609e-037	4.609e-037	-36.336	-36.336	0.000
TbF4-	0.000e+000	0.000e+000	-48.430	-48.599	-0.169
Tc(3)	0.000e+000				
Tc+3	0.000e+000	0.000e+000	-82.011	-83.523	-1.513
Tc(4)	0.000e+000				
TcO(OH)2	0.000e+000	0.000e+000	-47.554	-47.554	0.000
TcOOH+	0.000e+000	0.000e+000	-53.224	-53.394	-0.169
TcO+2	0.000e+000	0.000e+000	-59.585	-60.284	-0.700
(TcO(OH)2)2	0.000e+000	0.000e+000	-88.591	-88.591	0.000

Tc(5)	0.000e+000				
TcO4-3	0.000e+000	0.000e+000	-51.117	-52.819	-1.702
Tc(6)	6.619e-030				
HTcO4-	3.688e-030	2.498e-030	-29.433	-29.602	-0.169
TcO4-2	2.930e-030	5.283e-031	-29.533	-30.277	-0.744
H2TcO4	4.603e-038	4.603e-038	-37.337	-37.337	0.000
Tc(7)	6.088e-008				
TcO4-	6.088e-008	4.123e-008	-7.216	-7.385	-0.169
U(3)	0.000e+000				
U+3	0.000e+000	0.000e+000	-81.895	-83.408	-1.513
U(4)	1.199e-034				
U(OH)4	1.199e-034	1.199e-034	-33.921	-33.921	0.000
U(CO3)4-4	0.000e+000	0.000e+000	-45.777	-48.820	-3.043
U(CO3)5-6	0.000e+000	0.000e+000	-48.651	-55.526	-6.875
UOH+3	0.000e+000	0.000e+000	-52.493	-54.006	-1.513
U(SO4)2	0.000e+000	0.000e+000	-54.339	-54.339	0.000
USO4+2	0.000e+000	0.000e+000	-55.866	-56.565	-0.700
U+4	0.000e+000	0.000e+000	-58.921	-61.486	-2.565
UCl+3	0.000e+000	0.000e+000	-61.390	-62.902	-1.513
UNO3+3	0.000e+000	0.000e+000	-61.610	-63.123	-1.513
U(NO3)2+2	0.000e+000	0.000e+000	-64.700	-65.399	-0.700
UF+3	0.000e+000	0.000e+000	-65.050	-66.563	-1.513
UF2+2	0.000e+000	0.000e+000	-73.276	-73.975	-0.700
UI+3	0.000e+000	0.000e+000	-77.203	-78.716	-1.513
UF3+	0.000e+000	0.000e+000	-82.793	-82.962	-0.169
UF4	0.000e+000	0.000e+000	-93.357	-93.357	0.000
UF5-	0.000e+000	0.000e+000	-106.198	-106.367	-0.169
UF6-2	0.000e+000	0.000e+000	-117.931	-118.675	-0.744
USCN+3	0.000e+000	0.000e+000	-272.031	-273.544	-1.513
U(SCN)2+2	0.000e+000	0.000e+000	-486.579	-487.279	-0.700
U(5)	6.337e-025				
UO2+	6.337e-025	4.292e-025	-24.198	-24.367	-0.169
UO2(CO3)3-5	9.236e-030	1.578e-034	-29.035	-33.802	-4.767
U(6)	3.625e-006				
UO2(CO3)3-4	3.426e-006	3.103e-009	-5.465	-8.508	-3.043
UO2(CO3)2-2	1.606e-007	2.895e-008	-6.794	-7.538	-0.744
UO2(OH)2	2.890e-008	2.890e-008	-7.539	-7.539	0.000
UO2(OH)3-	5.611e-009	3.800e-009	-8.251	-8.420	-0.169
(UO2)2CO3(OH)3-	1.589e-009	1.076e-009	-8.799	-8.968	-0.169
UO2CO3	6.320e-010	6.320e-010	-9.199	-9.199	0.000
UO2PO4-	1.616e-010	1.095e-010	-9.792	-9.961	-0.169
UO2OH+	5.132e-011	3.476e-011	-10.290	-10.459	-0.169
UO2HPO4	2.327e-012	2.327e-012	-11.633	-11.633	0.000
UO2(SO4)2-2	1.873e-012	3.377e-013	-11.727	-12.471	-0.744
UO2SO4	1.565e-012	1.565e-012	-11.805	-11.805	0.000
UO2+2	2.648e-013	5.288e-014	-12.577	-13.277	-0.700
(UO2)3(CO3)6-6	2.591e-013	3.456e-020	-12.587	-19.461	-6.875
UO2(OH)4-2	3.489e-014	6.290e-015	-13.457	-14.201	-0.744
(UO2)3(OH)7-	2.959e-015	2.004e-015	-14.529	-14.698	-0.169
(UO2)3(OH)5+	7.514e-016	5.089e-016	-15.124	-15.293	-0.169
(UO2)2(OH)2+2	3.671e-016	7.333e-017	-15.435	-16.135	-0.700

UO2NO3+	1.219e-016	8.256e-017	-15.914	-16.083	-0.169
UO2Cl+	8.541e-017	5.784e-017	-16.069	-16.238	-0.169
UO2H2PO4+	5.443e-017	3.686e-017	-16.264	-16.433	-0.169
UO2IO3+	2.825e-018	1.913e-018	-17.549	-17.718	-0.169
(UO2)4(OH)7+	1.970e-019	1.334e-019	-18.706	-18.875	-0.169
(UO2)3(OH)4+2	1.109e-019	2.215e-020	-18.955	-19.655	-0.700
(UO2)2OH+3	1.898e-020	5.829e-022	-19.722	-21.234	-1.513
(UO2)3(OH)5CO2+	3.324e-021	2.251e-021	-20.478	-20.648	-0.169
(UO2)3O(OH)2(HCO3)+	2.719e-021	1.842e-021	-20.566	-20.735	-0.169
UO2Cl2	2.177e-021	2.177e-021	-20.662	-20.662	0.000
UO2(H2PO4)2	6.453e-022	6.453e-022	-21.190	-21.190	0.000
UO2F+	4.224e-023	2.861e-023	-22.374	-22.544	-0.169
UO2(IO3)2	2.457e-023	2.457e-023	-22.610	-22.610	0.000
UO2H3PO4+2	7.477e-025	1.493e-025	-24.126	-24.826	-0.700
UO2(H2PO4)(H3PO4)+	9.049e-029	6.129e-029	-28.043	-28.213	-0.169
UO2F2	3.939e-034	3.939e-034	-33.405	-33.405	0.000
UO2ClO3+	4.041e-039	2.737e-039	-38.394	-38.563	-0.169
UO2F3-	0.000e+000	0.000e+000	-45.307	-45.476	-0.169
(UO2)11(CO3)6(OH)12-2	0.000e+000	0.000e+000	-46.342	-47.086	-0.744
UO2SO3	0.000e+000	0.000e+000	-52.959	-52.959	0.000
UO2F4-2	0.000e+000	0.000e+000	-58.295	-59.039	-0.744
UO2(SO3)2-2	0.000e+000	0.000e+000	-97.493	-98.237	-0.744
UO2N3+	0.000e+000	0.000e+000	-110.736	-110.905	-0.169
UO2S2O3	0.000e+000	0.000e+000	-156.680	-156.680	0.000
UO2(N3)2	0.000e+000	0.000e+000	-209.363	-209.363	0.000
UO2SCN+	0.000e+000	0.000e+000	-226.733	-226.902	-0.169
UO2(N3)3-	0.000e+000	0.000e+000	-307.991	-308.160	-0.169
UO2(N3)4-2	0.000e+000	0.000e+000	-408.445	-409.189	-0.744
UO2(SCN)2	0.000e+000	0.000e+000	-442.106	-442.106	0.000
UO2(SCN)3-	0.000e+000	0.000e+000	-656.113	-656.282	-0.169
V(3)	8.393e-038				
V(OH)2+	8.393e-038	5.685e-038	-37.076	-37.245	-0.169
VOH+2	0.000e+000	0.000e+000	-40.913	-41.612	-0.700
VSO4+	0.000e+000	0.000e+000	-45.493	-45.662	-0.169
V+3	0.000e+000	0.000e+000	-45.865	-47.378	-1.513
V2(OH)2+4	0.000e+000	0.000e+000	-79.939	-82.504	-2.565
V(4)	9.925e-023				
VOOH+	9.572e-023	6.483e-023	-22.019	-22.188	-0.169
VOSO4	2.099e-024	2.099e-024	-23.678	-23.678	0.000
VO+2	1.430e-024	2.855e-025	-23.845	-24.544	-0.700
VOF+	1.935e-035	1.310e-035	-34.713	-34.883	-0.169
(VO)2(OH)2+2	9.842e-040	1.966e-040	-39.007	-39.706	-0.700
VOF2	0.000e+000	0.000e+000	-46.441	-46.441	0.000
V(5)	7.451e-003				
VO3OH-2	6.487e-003	1.170e-003	-2.188	-2.932	-0.744
HVO4-2	6.458e-004	1.164e-004	-3.190	-3.934	-0.744
H2VO4-	1.937e-004	1.312e-004	-3.713	-3.882	-0.169
VO2(OH)2-	1.237e-004	8.379e-005	-3.908	-4.077	-0.169
VO4-3	3.487e-008	6.926e-010	-7.458	-9.160	-1.702
VO(OH)3	7.777e-009	7.777e-009	-8.109	-8.109	0.000

VO2+	2.189e-013	1.482e-013	-12.660	-12.829	-0.169
VO2SO4-	2.026e-013	1.372e-013	-12.693	-12.863	-0.169
VO2HPO4-	2.366e-014	1.602e-014	-13.626	-13.795	-0.169
VO2(HPO4)2-3	7.593e-017	1.508e-018	-16.120	-17.822	-1.702
VO2F	1.523e-024	1.523e-024	-23.817	-23.817	0.000
VO2H2PO4	1.053e-026	1.053e-026	-25.978	-25.978	0.000
VO2F2-	2.976e-036	2.015e-036	-35.526	-35.696	-0.169
Yb(2)	1.960e-035				
Yb+2	1.960e-035	3.915e-036	-34.708	-35.407	-0.700
Yb(3)	2.001e-002				
YbCO3+	9.875e-003	6.688e-003	-2.005	-2.175	-0.169
Yb(CO3)2-	4.866e-003	3.296e-003	-2.313	-2.482	-0.169
YbSO4+	1.960e-003	1.328e-003	-2.708	-2.877	-0.169
Yb(SO4)2-	1.439e-003	9.744e-004	-2.842	-3.011	-0.169
YbPO4	8.516e-004	8.516e-004	-3.070	-3.070	0.000
Yb+3	4.253e-004	1.306e-005	-3.371	-4.884	-1.513
Yb(PO4)2-3	3.519e-004	6.990e-006	-3.454	-5.156	-1.702
YbOH+2	1.706e-004	3.408e-005	-3.768	-4.467	-0.700
YbO+	3.912e-005	2.650e-005	-4.408	-4.577	-0.169
YbO2H	2.083e-005	2.083e-005	-4.681	-4.681	0.000
YbO2-	5.188e-006	3.514e-006	-5.285	-5.454	-0.169
YbHPO4+	3.082e-006	2.088e-006	-5.511	-5.680	-0.169
YbHCO3+2	2.413e-006	4.819e-007	-5.617	-6.317	-0.700
YbNO3+2	9.308e-008	1.859e-008	-7.031	-7.731	-0.700
YbCl+2	7.390e-008	1.476e-008	-7.131	-7.831	-0.700
Yb(HPO4)2-	7.809e-009	5.289e-009	-8.107	-8.277	-0.169
YbH2PO4+2	3.591e-010	7.173e-011	-9.445	-10.144	-0.700
YbCl2+	6.349e-012	4.300e-012	-11.197	-11.367	-0.169
YbF+2	2.064e-014	4.123e-015	-13.685	-14.385	-0.700
YbCl3	1.013e-015	1.013e-015	-14.995	-14.995	0.000
YbCl4-	4.071e-019	2.758e-019	-18.390	-18.559	-0.169
YbF2+	1.073e-025	7.268e-026	-24.969	-25.139	-0.169
YbF3	1.656e-037	1.656e-037	-36.781	-36.781	0.000
YbF4-	0.000e+000	0.000e+000	-48.777	-48.946	-0.169
Zn	1.286e-004				
ZnSO4	7.071e-005	7.071e-005	-4.151	-4.151	0.000
Zn+2	5.409e-005	1.382e-005	-4.267	-4.859	-0.593
ZnOH+	2.377e-006	1.610e-006	-5.624	-5.793	-0.169
Zn(OH)2	7.322e-007	7.322e-007	-6.135	-6.135	0.000
ZnCO3	2.765e-007	2.765e-007	-6.558	-6.558	0.000
ZnHCO3+	2.621e-007	1.775e-007	-6.582	-6.751	-0.169
ZnSeO4	7.393e-008	7.393e-008	-7.131	-7.131	0.000
Zn(OH)Cl	3.100e-008	3.100e-008	-7.509	-7.509	0.000
ZnCl+	2.521e-008	1.707e-008	-7.598	-7.768	-0.169
ZnPO4-	1.755e-008	1.188e-008	-7.756	-7.925	-0.169
ZnHPO4	4.021e-009	4.021e-009	-8.396	-8.396	0.000
Zn(OH)3-	3.558e-010	2.410e-010	-9.449	-9.618	-0.169
ZnCl2	1.466e-011	1.466e-011	-10.834	-10.834	0.000
Zn(OH)4-2	2.420e-014	4.363e-015	-13.616	-14.360	-0.744
ZnCl3-	8.791e-015	5.954e-015	-14.056	-14.225	-0.169
ZnCl4-2	1.840e-016	3.318e-017	-15.735	-16.479	-0.744

ZnF+	1.323e-018	8.959e-019	-17.878	-18.048	-0.169
ZnH2PO4+	8.150e-020	5.520e-020	-19.089	-19.258	-0.169
ZnI+	7.104e-027	4.812e-027	-26.148	-26.318	-0.169
ZnClO4+	3.495e-030	2.367e-030	-29.457	-29.626	-0.169
ZnI2	0.000e+000	0.000e+000	-43.593	-43.593	0.000
ZnI3-	0.000e+000	0.000e+000	-62.030	-62.200	-0.169
Zn(NH3)+2	0.000e+000	0.000e+000	-68.116	-68.816	-0.700
ZnI4-2	0.000e+000	0.000e+000	-80.500	-81.244	-0.744
ZnN3+	0.000e+000	0.000e+000	-104.456	-104.625	-0.169
Zn(NH3)2+2	0.000e+000	0.000e+000	-131.919	-132.619	-0.700
Zn(NH3)3+2	0.000e+000	0.000e+000	-195.722	-196.421	-0.700
Zn(N3)2	0.000e+000	0.000e+000	-204.080	-204.080	0.000
Zn(NH3)4+2	0.000e+000	0.000e+000	-259.798	-260.498	-0.700
Zn(SCN)2	0.000e+000	0.000e+000	-434.051	-434.051	0.000
Zn(CN)4-2	0.000e+000	0.000e+000	-481.541	-482.285	-0.744
Zn(SCN)4-2	0.000e+000	0.000e+000	-863.011	-863.755	-0.744

----------Saturation indices----------

Phase	SI	log IAP	log KT	
(UO2)2As2O7	-77.27	-69.59	7.68	(UO2)2As2O7
(UO2)2Cl3	-59.72	-48.53	11.20	(UO2)2Cl3
(UO2)2P2O7	-25.37	-40.14	-14.77	(UO2)2P2O7
(UO2)3(AsO4)2	-76.10	-66.80	9.29	(UO2)3(AsO4)2
(UO2)3(PO4)2	-23.26	-37.36	-14.10	(UO2)3(PO4)2
(UO2)3(PO4)2:4H2O	-10.33	-37.38	-27.05	(UO2)3(PO4)2:4H2O
(VO)3(PO4)2	-119.95	-121.90	-1.96	(VO)3(PO4)2
Afwillite	-28.58	31.39	59.96	Ca3Si2O4(OH)6
Akermanite	-15.00	30.23	45.23	Ca2MgSi2O7
Al	-139.83	-54.41	85.42	Al
Al(g)	-190.53	-54.41	136.12	Al
Al2(SO4)3	-57.13	-38.23	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-39.82	-38.27	1.56	Al2(SO4)3:6H2O
Alabandite	-145.52	-179.65	-34.13	MnS
Albite	0.00	2.66	2.66	NaAlSi3O8
Albite_high	-1.32	2.66	3.98	NaAlSi3O8
Albite_low	-0.00	2.66	2.66	NaAlSi3O8
AlF3	-42.44	-59.71	-17.27	AlF3
Alstonite	-4.43	-1.84	2.58	BaCa(CO3)2
Alum-K	-18.74	-23.72	-4.97	KAl(SO4)2:12H2O
Alunite	-8.40	-8.87	-0.47	KAl3(OH)6(SO4)2
Amesite-14A	-5.87	69.40	75.27	Mg4Al4Si2O10(OH)8
Analcime	-0.13	5.93	6.06	Na.96Al.96Si2.04O6:H2O
Analcime-dehy	-6.49	5.93	12.42	Na.96Al.96Si2.04O6
Andalusite	-5.12	10.76	15.88	Al2SiO5
Andradite	5.49	64.71	59.22	Ca3Fe2(SiO4)3
Anhydrite	-0.17	-4.52	-4.35	CaSO4
Annite	-35.52	-6.19	29.33	KFe3AlSi3O10(OH)2
Anorthite	-6.59	19.88	26.48	CaAl2(SiO4)2
Antarcticite	-13.30	-9.21	4.09	CaCl2:6H2O

Anthophyllite	-14.87	51.61	66.48	Mg7Si8O22(OH)2
Antigorite	-37.86	437.77	475.63	Mg48Si34O85(OH)62
Aphthitalite	-11.17	-15.06	-3.89	NaK3(SO4)2
Aragonite	-0.15	1.82	1.97	CaCO3
Arcanite	-7.21	-9.05	-1.84	K2SO4
Arsenolite	-112.78	-157.55	-44.77	As2O3
Arsenopyrite	-262.21	-324.99	-62.78	FeAsS
Artinite	-7.03	12.60	19.63	Mg2CO3(OH)2:3H2O
As	-106.30	-140.58	-34.28	As
As2O5	-77.28	-75.15	2.14	As2O5
As4O6(cubi)	-225.42	-315.10	-89.69	As4O6
As4O6(mono)	-225.19	-315.10	-89.91	As4O6
Autunite-H	-14.79	-40.15	-25.35	H2(UO2)2(PO4)2
B	-107.51	-62.45	45.06	B
B(g)	-198.80	-62.45	136.35	B
B2O3	-6.84	-1.30	5.55	B2O3
Ba	-131.77	-33.54	98.23	Ba
Ba(OH)2:8H2O	-16.89	7.60	24.49	Ba(OH)2:8H2O
Ba2Si3O8	-19.99	3.24	23.23	Ba2Si3O8
Ba2SiO4	-33.26	11.29	44.55	Ba2SiO4
Ba2U2O7	-53.81	-20.32	33.49	Ba2U2O7
Ba3UO6	-68.60	25.76	94.36	Ba3UO6
BaCl2	-16.89	-14.67	2.23	BaCl2
BaCl2:2H2O	-14.89	-14.68	0.21	BaCl2:2H2O
BaCl2:H2O	-15.50	-14.67	0.82	BaCl2:H2O
BaHPO4	-7.79	-15.19	-7.40	BaHPO4
BaI2	-56.33	-267.94	-211.61	BaI2
BaMnO4	-15.47	92.89	108.36	BaMnO4
BaO	-40.14	7.66	47.80	BaO
Barite	0.00	-10.01	-10.01	BaSO4
Barytocalcite	-4.59	-1.84	2.74	BaCa(CO3)2
BaS	-157.35	-174.82	-17.47	BaS
BaSeO3	-18.47	-54.06	-35.59	BaSeO3
BaSeO4	-5.40	-12.86	-7.46	BaSeO4
BaSiF6	-98.36	-130.57	-32.22	BaSiF6
Bassanite	-0.82	-4.52	-3.71	CaSO4:0.5H2O
Bassetite	-24.33	-42.07	-17.74	Fe(UO2)2(PO4)2
BaU2O7	-8.74	13.22	21.96	BaU2O7
BaUO4	-7.75	10.44	18.19	BaUO4
Beidellite-Ca	-0.84	4.61	5.44	Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H	-2.05	2.44	4.49	H.33Al2.33Si3.67O10(OH)2
Beidellite-K	-1.30	3.86	5.16	K.33Al2.33Si3.67O10(OH)2
Beidellite-Mg	-0.99	4.41	5.41	Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na	-0.64	4.86	5.50	Na.33Al2.33Si3.67O10(OH)2
Berlinite	-8.19	-15.46	-7.27	AlPO4
BF3(g)	-64.77	-67.75	-2.98	BF3

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      Birnessite          0.00  269.79  269.79  Mn8O14:5H2O
      Bischofite        -14.78  -10.39    4.39  MgCl2:6H2O
      Bixbyite           -3.33   46.86   50.18  Mn2O3
      Bloedite           -6.22   -8.70   -2.48  Na2Mg(SO4)2:4H2O
      Boehmite           -0.16    7.39    7.55  AlO2H
      Boltwoodite       -11.83    3.06   14.89  K(H3O)(UO2)SiO4
      Boltwoodite-Na     -9.41    5.18   14.58
Na.7K.3(H3O)(UO2)SiO4:H2O
      Borax              -0.00   12.04   12.04  Na2(B4O5(OH)4):8H2O
      Boric_acid         -0.50   -0.66   -0.16  B(OH)3
      Brucite            -4.31   11.97   16.28  Mg(OH)2
      Brushite          -16.26   -9.71    6.55  CaHPO4:2H2O
      Burkeite          -12.07   -2.58    9.49  Na6CO3(SO4)2
      C                 -71.88  -93.73  -21.85  C
      C(g)             -189.50  -93.73   95.77  C
      Ca               -124.88  -28.05   96.83  Ca
      Ca(g)            -150.12  -28.05  122.07  Ca
      Ca-Al_Pyroxene    -11.99   23.91   35.90  CaAl2SiO6
      Ca2Al2O5:8H2O     -18.53   41.04   59.57  Ca2Al2O5:8H2O
      Ca2Cl2(OH)2:H2O   -22.32    3.97   26.29  Ca2Cl2(OH)2:H2O
      Ca2V2O7            -0.47   16.71   17.18  Ca2V2O7
      Ca3(AsO4)2        -53.49  -35.69   17.80  Ca3(AsO4)2
      Ca3Al2O6          -58.79   54.25  113.03  Ca3Al2O6
      Ca3V2O8            -8.71   29.86   38.57  Ca3V2O8
      Ca4Al2Fe2O10      -61.79  104.73  166.52  Ca4Al2Fe2O10
      Ca4Al2O7:13H2O    -39.94   67.32  107.25  Ca4Al2O7:13H2O
      Ca4Al2O7:19H2O    -36.40   67.28  103.68  Ca4Al2O7:19H2O
      Ca4Cl2(OH)6:13H2O -38.14   30.19   68.33  Ca4Cl2(OH)6:13H2O
      CaAl2O4           -18.97   27.94   46.91  CaAl2O4
      CaAl2O4:10H2O     -10.12   27.88   37.99  CaAl2O4:10H2O
      CaAl4O7           -25.87   42.73   68.59  CaAl4O7
      Calcite            -0.00    1.82    1.82  CaCO3
      Carnallite        -21.51  -17.24    4.27  KMgCl3:6H2O
      Carnotite           4.07    4.59    0.51  K2(UO2)2(VO4)2
      CaSeO3:2H2O       -14.93  -48.58  -33.65  CaSeO3:2H2O
      CaSeO4             -4.28   -7.37   -3.09  CaSeO4
      CaSO4:0.5H2O(beta)  -0.99   -4.52   -3.54  CaSO4:0.5H2O
      CaUO4               0.00   15.94   15.94  CaUO4
      CaV2O6             -1.98    3.55    5.53  CaV2O6
      Celadonite          0.25    7.56    7.31  KMgAlSi4O10(OH)2
      CH4(g)           -145.41 -176.15  -30.74  CH4
      Chalcedony         -0.27   -4.03   -3.76  SiO2
      Chamosite-7A      -25.88    6.88   32.76  Fe2Al2SiO5(OH)4
      Chloromagnesite   -32.16  -10.35   21.82  MgCl2
      Chrysotile         -3.17   27.86   31.03  Mg3Si2O5(OH)4
      Cl2(g)            -27.12   18.88   45.99  Cl2

      Claudetite       -112.83 -157.55  -44.73  As2O3
      Clinochlore-14A    -4.49   62.56   67.05  Mg5Al2Si3O10(OH)8
      Clinochlore-7A     -7.86   62.56   70.42  Mg5Al2Si3O10(OH)8
      Clinoptilolite-Ca  -2.69   -9.98   -7.29
Ca1.7335Al3.45Fe.017Si14.533O36:10.922H2O
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      Clinoptilolite-dehy-Ca -38.27   -9.91   28.36
 Ca1.7335Al3.45Fe.017Si14.533O36
      Clinoptilolite-dehy-K -42.19  -17.77   24.43
 K3.467Al3.45Fe.017Si14.533O36
      Clinoptilolite-dehy-Na -35.47   -7.24   28.23
 Na3.467Al3.45Fe.017Si14.533O36
      Clinoptilolite-dehy-NH4-254.96 -642.68 -387.72
 (NH4)3.467Al3.45Fe.017Si14.533O36
      Clinoptilolite-hy-Ca  -2.69   -9.99   -7.29
 Ca1.7335Al3.45Fe.017Si14.533O36:11.645H2O
      Clinoptilolite-hy-K  -6.58  -17.81  -11.23
 K3.467Al3.45Fe.017Si14.533O36:7.499H2O
      Clinoptilolite-hy-Na   0.12   -7.31   -7.43
 Na3.467Al3.45Fe.017Si14.533O36:10.877H2O
      Clinoptilolite-K  -6.61  -17.84  -11.23
 K3.467Al3.45Fe.017Si14.533O36:10.922H2O
      Clinoptilolite-Na   0.12   -7.31   -7.42
 Na3.467Al3.45Fe.017Si14.533O36:10.922H2O
      Clinoptilolite-NH4-219.39 -642.75 -423.36
 (NH4)3.467Al3.45Fe.017Si14.533O36:10.922H2O
      Clinozoisite     -6.70   36.40   43.10  Ca2Al3Si3O12(OH)
      CO(g)           -48.21  -52.53   -4.32  CO
      CO2(g)           -3.50  -11.33   -7.83  CO2
      Coesite          -0.81   -4.03   -3.22  SiO2
      Coffinite       -25.33  -42.45  -17.12  USiO4
      Colemanite        0.87   22.39   21.51  Ca2B6O11:5H2O
      Cordierite_anhyd -18.68   33.39   52.07  Mg2Al4Si5O18
      Cordierite_hydr -16.20   33.38   49.59  Mg2Al4Si5O18:H2O
      Corundum         -3.50   14.79   18.29  Al2O3
      Cristobalite(alpha)  -0.55   -4.03   -3.48  SiO2
      Cristobalite(beta)  -0.99   -4.03   -3.03  SiO2
      Cronstedtite-7A -12.79   29.43   42.21  Fe2Fe2SiO5(OH)4
      Daphnite-14A    -59.09   -6.99   52.10  Fe5AlAlSi3O10(OH)8
      Daphnite-7A     -62.47   -6.99   55.48  Fe5AlAlSi3O10(OH)8
      Dawsonite        -0.93    3.41    4.34  NaAlCO3(OH)2
      Diaspore          0.24    7.39    7.15  AlHO2
      Dicalcium_silicate -14.85   22.28   37.13  Ca2SiO4
      Diopside         -3.81   17.07   20.89  CaMgSi2O6
      Dolomite         -0.00    2.47    2.47  CaMg(CO3)2
      Dolomite-dis     -1.54    2.47    4.01  CaMg(CO3)2
      Dolomite-ord      0.01    2.47    2.46  CaMg(CO3)2
      Downeyite       -25.92  -61.72  -35.81  SeO2
      Enstatite        -3.34    7.95   11.29  MgSiO3
      Epidote           1.88   47.67   45.79  Ca2FeAl2Si3O12OH
      Epidote-ord       1.89   47.67   45.78  FeCa2Al2(OH)(SiO4)3
      Epsomite         -3.78   -5.74   -1.96  MgSO4:7H2O
      Ettringite      -21.98   40.49   62.46
 Ca6Al2(SO4)3(OH)12:26H2O
      F2(g)          -102.24   -3.53   98.71  F2
      Fayalite        -26.96   -7.90   19.06  Fe2SiO4
      Fe              -59.15  -43.13   16.02  Fe
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Fe(OH)2	-15.83	-1.94	13.89	Fe(OH)2
Fe(OH)3	0.00	18.66	18.66	Fe(OH)3
Fe2(SO4)3	-44.77	-15.68	29.08	Fe2(SO4)3
FeF2	-44.24	-46.67	-2.42	FeF2
FeF3	-42.20	-48.44	-6.24	FeF3
FeO	-15.46	-1.93	13.52	FeO
Ferrite-Ca	2.96	50.49	47.53	CaFe2O4
Ferrite-Dicalcium	-19.19	63.64	82.84	Ca2Fe2O5
Ferrite-Mg	2.25	49.31	47.06	MgFe2O4
Ferrite-Zn	10.80	48.53	37.74	ZnFe2O4
Ferroselite	-152.57	-331.38	-178.81	FeSe2
Ferrosilite	-13.37	-5.96	7.41	FeSiO3
FeSO4	-22.21	-19.61	2.61	FeSO4
FeV2O4	-329.07	-93.94	235.14	FeV2O4
Fluorapatite	-0.00	-25.16	-25.16	Ca5(PO4)3F
Fluorite	-21.51	-31.58	-10.07	CaF2
Forsterite	-7.88	19.93	27.81	Mg2SiO4
Foshagite	-25.28	40.52	65.80	Ca4Si3O9(OH)2:0.5H2O
Frankdicksonite	-31.32	-37.08	-5.76	BaF2
Gaylussite	-6.00	5.16	11.16	CaNa2(CO3)2:5H2O
Gehlenite	-19.16	37.06	56.22	Ca2Al2SiO7
Gibbsite	-0.36	7.38	7.74	Al(OH)3
Gismondine	-2.01	39.71	41.72	Ca2Al4Si4O16:9H2O
Glauberite	-2.03	-7.49	-5.47	Na2Ca(SO4)2
Goethite	5.12	18.66	13.55	FeOOH
Greenalite	-36.45	-13.87	22.58	Fe3Si2O5(OH)4
Grossular	-9.61	42.16	51.78	Ca3Al2(SiO4)3
Gypsum	0.00	-4.53	-4.53	CaSO4:2H2O
Gyrolite	-8.60	14.21	22.80	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-41.21	-41.21	-0.00	H2
H2O(g)	-1.59	-0.01	1.59	H2O
H2S(g)	-140.78	-182.48	-41.70	H2S
Haiweeite	1.56	-5.48	-7.04	Ca(UO2)2(Si2O5)3:5H2O
Halite	-5.38	-3.81	1.56	NaCl
Hatrurite	-37.92	35.43	73.35	Ca3SiO5
Hausmannite	-11.61	49.68	61.29	Mn3O4
HCl(g)	-17.47	-11.17	6.30	HCl
Hedenbergite	-16.36	3.16	19.53	CaFe(SiO3)2
Hematite	11.22	37.33	26.11	Fe2O3
Hercynite	-15.95	12.85	28.80	FeAl2O4
Hexahydrite	-4.01	-5.73	-1.73	MgSO4:6H2O
HI(g)	-35.87	-137.80	-101.93	HI
Hillebrandite	-14.50	22.27	36.77	Ca2SiO3(OH)2:0.17H2O
Hopeite	-1.47	-12.13	-10.66	Zn3(PO4)2:4H2O
HTcO4	-21.37	-15.42	5.95	HTcO4
Huntite	-6.45	3.77	10.22	CaMg3(CO3)4
Hydroboracite	0.84	21.20	20.36	MgCaB6O11:6H2O
Hydromagnesite	-16.20	14.54	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.92	-9.17	11.75	CaCl2
Hydroxylapatite	0.43	-2.79	-3.22	Ca5(OH)(PO4)3
Hydrozincite	3.01	33.32	30.31	Zn5(OH)6(CO3)2
I2	-29.91	-234.40	-204.49	I2

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      I2(g)            -33.32 -234.40 -201.08  I2
      Ice               -0.15   -0.01    0.14  H2O
      Illite            -0.40    8.48    8.88
K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
      Jadeite           -1.62    6.69    8.31  NaAl(SiO3)2
      Jarosite          -4.70   24.95   29.64  KFe3(SO4)2(OH)6
      Jarosite-Na       -5.62   27.99   33.61  NaFe3(SO4)2(OH)6
      K                -65.77  -16.29   49.48  K
      K(g)             -76.37  -16.29   60.08  K
      K-Feldspar        -0.00   -0.38   -0.38  KAlSi3O8
      K2CO3:1.5H2O     -16.09   -2.72   13.38  K2CO3:1.5H2O
      K2O              -75.41    8.62   84.04  K2O
      K2Se            -121.74 -176.70  -54.97  K2Se
      K2UO4            -22.47   11.40   33.87  K2UO4
      K3H(SO4)2        -18.79  -22.41   -3.62  K3H(SO4)2
      K8H4(CO3)6:3H2O  -61.22  -33.51   27.71  K8H4(CO3)6:3H2O
      Kainite          -12.25  -12.57   -0.31  KMgClSO4:3H2O
      KAl(SO4)2        -26.91  -23.64    3.27  KAl(SO4)2
      Kalicinite        -7.30   -7.02    0.28  KHCO3
      Kalsilite         -3.17    7.68   10.85  KAlSiO4
      Kaolinite          0.00    6.72    6.72  Al2Si2O5(OH)4
      Karelianite      -56.53  -92.00  -35.47  V2O3
      Katoite          -24.74   54.21   78.94  Ca3Al2H12O12
      Kieserite         -5.43   -5.70   -0.27  MgSO4:H2O
      KMgCl3           -38.45  -17.20   21.25  KMgCl3
      KMgCl3:2H2O      -31.17  -17.21   13.96  KMgCl3:2H2O
      KNaCO3:6H2O       -9.97    0.29   10.26  KNaCO3:6H2O
      KTcO4             -8.83  -11.10   -2.27  KTcO4
      KUO2AsO4         -26.31  -30.48   -4.17  KUO2AsO4
      Kyanite           -4.85   10.76   15.61  Al2SiO5
      Lansfordite       -4.22    0.62    4.84  MgCO3:5H2O
      Larnite          -16.14   22.28   38.42  Ca2SiO4
      Laumontite        -1.71   11.80   13.51  CaAl2Si4O12:4H2O
      Lawrencite       -33.31  -24.26    9.05  FeCl2
      Lawsonite         -2.23   19.87   22.11  CaAl2Si2O7(OH)2:H2O
      Leonite          -10.66  -14.77   -4.11  K2Mg(SO4)2:4H2O
      Lime             -19.42   13.15   32.57  CaO
      Magnesite         -1.62    0.65    2.27  MgCO3
      Magnetite         -1.05   35.40   36.45  Fe3O4
      Manganite         -1.98   23.42   25.41  MnO(OH)
      Manganosite      -15.09    2.83   17.92  MnO
      Margarite         -6.26   34.66   40.93  CaAl4Si2O10(OH)2
      Maximum_Microcline   0.00   -0.38   -0.38  KAlSi3O8
      Mayenite       -232.81  261.34  494.15  Ca12Al14O33
      Melanterite      -17.25  -19.65   -2.40  FeSO4:7H2O
      Mercallite       -11.93  -13.36   -1.44  KHSO4
      Merwinite        -25.03   43.38   68.41  MgCa3(SiO4)2


      Mesolite           2.69   16.18   13.49
Na.676Ca.657Al1.99Si3.01O10:2.647H2O
      Mg               -108.75  -29.22   79.52  Mg
      Mg(g)            -128.47  -29.22   99.25  Mg
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      Mg1.25SO4(OH)0.5:0.5H2O  -7.90   -2.71    5.20
Mg1.25SO4(OH)0.5:0.5H2O
      Mg1.5SO4(OH)     -8.92    0.29    9.21  Mg1.5SO4(OH)
      Mg2V2O7         -11.64   14.36   25.99  Mg2V2O7
      MgCl2:2H2O      -23.09  -10.36   12.73  MgCl2:2H2O
      MgCl2:4H2O      -17.68  -10.37    7.30  MgCl2:4H2O
      MgCl2:H2O       -26.43  -10.35   16.07  MgCl2:H2O
      MgOHCl          -15.08    0.81   15.89  MgOHCl
      MgSeO3          -22.40  -49.74  -27.34  MgSeO3
      MgSeO3:6H2O     -17.33  -49.78  -32.45  MgSeO3:6H2O
      MgSO4           -10.52   -5.69    4.83  MgSO4
      MgUO4            -8.23   14.76   22.99  MgUO4
      MgV2O6           -8.67    2.38   11.05  MgV2O6
      Minnesotaite    -35.75  -21.92   13.83  Fe3Si4O10(OH)2
      Mirabilite       -1.88   -3.04   -1.15  Na2SO4:10H2O
      Misenite        -78.16  -89.23  -11.08  K8H6(SO4)7
      Mn              -78.31  -38.37   39.94  Mn
      Mn(OH)2(am)     -12.49    2.82   15.31  Mn(OH)2
      Mn(OH)3          -8.50   23.42   31.92  Mn(OH)3
      Mn3(PO4)2       -38.04  -37.22    0.82  Mn3(PO4)2
      MnCl2:2H2O      -23.51  -19.51    4.00  MnCl2:2H2O
      MnCl2:4H2O      -22.28  -19.52    2.75  MnCl2:4H2O
      MnCl2:H2O       -25.05  -19.50    5.54  MnCl2:H2O
      MnHPO4           -7.08  -20.03  -12.95  MnHPO4
      MnO2(gamma)       0.93   44.03   43.10  MnO2
      MnSe           -105.55 -182.50  -76.95  MnSe
      MnSeO3          -22.61  -58.89  -36.29  MnSeO3
      MnSeO3:2H2O     -23.56  -58.91  -35.35  MnSeO3:2H2O
      MnSO4           -17.45  -14.84    2.61  MnSO4
      MnV2O6          -11.59   -6.77    4.82  MnV2O6
      Molysite        -41.31  -14.82   26.49  FeCl3
      Monohydrocalcite  -0.86    1.82    2.68  CaCO3:H2O
      Monticellite     -8.43   21.10   29.53  CaMgSiO4
      Montmor-Ca        0.01    2.35    2.34
Ca.165Mg.33Al1.67Si4O10(OH)2
      Montmor-K        -0.39    1.60    1.99
K.33Mg.33Al1.67Si4O10(OH)2
      Montmor-Mg       -0.08    2.16    2.23
Mg.495Al1.67Si4O10(OH)2
      Montmor-Na        0.28    2.61    2.33
Na.33Mg.33Al1.67Si4O10(OH)2
      Mordenite        -1.63   -6.99   -5.36
Ca.2895Na.361Al.94Si5.06O12:3.468H2O
      Mordenite-dehy  -16.74   -6.97    9.77
Ca.2895Na.361Al.94Si5.06O12
      Muscovite         0.95   14.40   13.45  KAl3Si3O10(OH)2
      N2(g)           -17.75 -228.24 -210.49  N2
      Na              -59.12  -13.25   45.87  Na


      Na(g)           -72.61  -13.25   59.36  Na
      Na2CO3           -7.80    3.37   11.16  Na2CO3
      Na2CO3:7H2O      -6.62    3.32    9.94  Na2CO3:7H2O
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Na2O	-52.72	14.70	67.42	Na2O
Na2Se	-116.21	-170.63	-54.42	Na2Se
Na2Se2	-163.89	-314.75	-150.86	Na2Se2
Na2SiO3	-11.53	10.67	22.20	Na2SiO3
Na2U2O7	-2.33	20.26	22.59	Na2U2O7
Na2UO4(alpha)	-12.54	17.48	30.02	Na2UO4
Na3H(SO4)2	-12.41	-13.30	-0.89	Na3H(SO4)2
Na3UO4	-50.53	4.23	54.76	Na3UO4
Na4Ca(SO4)3:2H2O	-4.59	-10.48	-5.89	Na4Ca(SO4)3:2H2O
Na4SiO4	-45.23	25.36	70.60	Na4SiO4
Na4UO2(CO3)3	-5.85	-1.81	4.04	Na4UO2(CO3)3
Na6Si2O7	-65.50	36.03	101.53	Na6Si2O7
NaFeO2	-6.89	26.02	32.90	NaFeO2
Nahcolite	-3.84	-3.98	-0.14	NaHCO3
NaTcO4	-9.59	-8.07	1.52	NaTcO4
Natrolite	-1.00	17.39	18.39	Na2Al2Si3O10:2H2O
Natron	-6.28	3.30	9.59	Na2CO3:10H2O
Natrosilite	-11.42	6.64	18.07	Na2Si2O5
NaUO3	-17.32	-10.47	6.85	NaUO3
Nepheline	-3.04	10.71	13.75	NaAlSiO4
Nesquehonite	-4.66	0.63	5.29	MgCO3:3H2O
NH3(g)	-67.81	-175.93	-108.13	NH3
NH4HSe	-163.03	-361.26	-198.23	NH4HSe
Ningyoite	-32.12	-70.98	-38.86	CaUP2O8:2H2O
Niter	-6.58	-6.81	-0.22	KNO3
Nitrobarite	-12.08	-14.57	-2.49	Ba(NO3)2
NO(g)	-24.39	-72.92	-48.53	NO
NO2(g)	-18.57	-31.72	-13.15	NO2
Nontronite-Ca	12.85	27.16	14.31	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	11.64	24.98	13.35	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	12.38	26.41	14.02	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	12.69	26.96	14.27	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	13.05	27.41	14.36	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-0.70	82.40	83.10	O2
Okenite	-5.23	5.09	10.31	CaSi2O4(OH)2:H2O
Orpiment	-499.45	-704.98	-205.54	As2S3
Oxychloride-Mg	-13.07	12.76	25.83	Mg2Cl(OH)3:4H2O
P	-150.41	-125.85	24.56	P
Paragonite	0.06	17.44	17.38	NaAl3Si3O10(OH)2
Pargasite	-22.13	79.57	101.70	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrite	-4.34	-5.73	-1.39	MgSO4:5H2O
Periclase	-9.35	11.98	21.33	MgO
Phlogopite	-1.75	35.55	37.30	KAlMg3Si3O10(OH)2
Picromerite	-10.34	-14.78	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-6.14	5.18	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-9.48	-23.79	-14.31	K2MgCa2(SO4)4:2H2O

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      Portlandite      -9.40   13.15   22.55  Ca(OH)2
      Prehnite         -3.79   29.00   32.79  Ca2Al2Si3O10(OH)2
      Pseudowollastonite  -4.84    9.13   13.96  CaSiO3
      Pu             -174.14 -108.33   65.81  Pu
      Pu(HPO4)2       -25.31  -71.64  -46.33  Pu(HPO4)2
      Pu(OH)3         -33.43  -46.54  -13.11  Pu(OH)3
      Pu(OH)4          -8.14  -25.94  -17.81  Pu(OH)4
      Pu2O3           -70.07  -93.06  -22.98  Pu2O3
      PuF3            -67.83 -113.63  -45.80  PuF3
      PuF4            -83.55 -115.40  -31.85  PuF4
      PuO2              0.00  -25.93  -25.93  PuO2
      PuO2(OH)2        -4.59   15.27   19.86  PuO2(OH)2
      PuO2HPO4        -11.24   -7.58    3.66  PuO2HPO4
      PuO2OH(am)      -10.79   -5.33    5.46  PuO2OH
      Pyrite         -242.00 -325.69  -83.69  FeS2
      Pyrolusite        2.47   44.03   41.56  MnO2
      Pyrophyllite     -1.62   -1.33    0.29  Al2Si4O10(OH)2
      Pyrrhotite     -146.96 -184.41  -37.45  FeS
      Quartz            0.00   -4.03   -4.03  SiO2
      Rankinite       -20.42   31.40   51.82  Ca3Si2O7
      Realgar        -200.74 -281.85  -81.11  AsS
      Rhodochrosite    -8.28   -8.50   -0.22  MnCO3
      Rhodonite       -10.89   -1.20    9.69  MnSiO3
      Ripidolite-14A  -26.04   34.74   60.78  Mg3Fe2Al2Si3O10(OH)8
      Ripidolite-7A   -29.42   34.74   64.16  Mg3Fe2Al2Si3O10(OH)8
      Rutherfordine    -4.43   -8.55   -4.12  UO2CO3
      S              -105.46 -141.28  -35.82  S
      S2(g)          -224.80 -282.55  -57.75  S2
      Saleeite         -8.69  -28.16  -19.48  Mg(UO2)2(PO4)2
      Sanbornite       -9.80   -0.40    9.41  BaSi2O5
      Sanidine_high    -1.20   -0.38    0.82  KAlSi3O8
      Saponite-Ca      -0.39   25.75   26.14
Ca.165Mg3Al.33Si3.67O10(OH)2
      Saponite-H       -1.60   23.58   25.18
H.33Mg3Al.33Si3.67O10(OH)2
      Saponite-K       -0.85   25.01   25.86
K.33Mg3Al.33Si3.67O10(OH)2
      Saponite-Mg      -0.54   25.56   26.10
Mg3.165Al.33Si3.67O10(OH)2
      Saponite-Na      -0.19   26.01   26.20
Na.33Mg3Al.33Si3.67O10(OH)2
      Scacchite       -28.24  -19.50    8.74  MnCl2
      Schoepite        -2.07    2.77    4.83  UO3:2H2O
      Schoepite-dehy(.393)  -3.95    2.78    6.72  UO3:.393H2O
      Schoepite-dehy(.648)  -3.43    2.78    6.21  UO3:.648H2O
      Schoepite-dehy(.85)  -2.32    2.78    5.10  UO3:.85H2O
      Schoepite-dehy(.9)  -2.24    2.78    5.02  UO3:.9H2O
      Schoepite-dehy(1.0)  -2.33    2.78    5.10  UO3:H2O
      Scolecite         0.09   15.84   15.75  CaAl2Si3O10:3H2O
      Se             -55.21 -144.12  -88.92  Se
      Se2O5          -62.72  -82.24  -19.53  Se2O5
      SeCl4          -91.69 -106.37  -14.68  SeCl4
      Sellaite       -23.31  -32.76   -9.44  MgF2
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SeO3	-39.68	-20.52	19.16	SeO3
Sepiolite	-6.52	23.70	30.22	Mg4Si6O15(OH)2:6H2O
Shcherbinaite	-8.15	-9.60	-1.45	V2O5
Si	-149.30	-86.43	62.87	Si
Si(g)	-220.37	-86.43	133.94	Si
Siderite	-13.04	-13.26	-0.22	FeCO3
SiF4(g)	-78.26	-93.50	-15.24	SiF4
Sillimanite	-5.49	10.76	16.24	Al2SiO5
SiO2(am)	-1.29	-4.03	-2.74	SiO2
Sklodowskite	-4.35	9.44	13.79	Mg(H3O)2(UO2)2(SiO4)2:4H2O
Smectite-high-Fe-Mg	-6.27	13.60	19.88	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	-3.41	9.56	12.98	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
Smithsonite	-0.57	-0.13	0.44	ZnCO3
SO2(g)	-53.56	-58.87	-5.32	SO2
Soddyite	1.13	1.52	0.39	(UO2)2SiO4:2H2O
Sphalerite	-126.10	-171.28	-45.18	ZnS
Spinel	-10.84	26.76	37.61	Al2MgO4
Starkeyite	-4.72	-5.72	-1.00	MgSO4:4H2O
Stilbite	2.22	3.03	0.81	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Stilleite	-83.89	-174.13	-90.24	ZnSe
Strengite	-5.82	-4.20	1.63	FePO4:2H2O
Sylvite	-7.68	-6.85	0.83	KCl
Syngenite	-5.97	-13.57	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-47.09	-29.94	17.14	Mg2CaCl6:12H2O
Talc	-1.17	19.81	20.99	Mg3Si4O10(OH)2
Tb	-158.69	-41.80	116.89	Tb
Tb(OH)3	4.31	19.99	15.69	Tb(OH)3
Tb(OH)3(am)	1.21	19.99	18.79	Tb(OH)3
Tb2(CO3)3	9.24	6.02	-3.21	Tb2(CO3)3
Tb2O3	-7.09	40.01	47.10	Tb2O3
TbF3:.5H2O	-30.40	-47.10	-16.70	TbF3:.5H2O
TbPO4:10H2O	9.07	-2.91	-11.98	TbPO4:10H2O
Tc	-102.70	-159.62	-56.92	Tc
Tc(OH)2	-63.82	-118.42	-54.61	Tc(OH)2
Tc(OH)3	-50.20	-97.83	-47.62	Tc(OH)3
Tc2O7	-43.93	-30.83	13.10	Tc2O7
Tc2O7(g)	-52.18	-30.83	21.35	Tc2O7
Tc2S7	-841.94	-1308.17	-466.23	Tc2S7
Tc3O4	-158.18	-314.05	-155.87	Tc3O4
Tc4O7	-181.31	-350.07	-168.76	Tc4O7
TcO2:2H2O(am)	-40.01	-77.23	-37.22	TcO2:2H2O
TcO3	-23.19	-36.01	-12.83	TcO3
TcOH	-82.54	-139.02	-56.48	TcOH
TcS2	-275.79	-442.17	-166.38	TcS2
TcS3	-373.14	-583.45	-210.30	TcS3
Tephroite	-21.40	1.63	23.02	Mn2SiO4
Thenardite	-2.62	-2.98	-0.36	Na2SO4

Thermonatrite	-7.58	3.36	10.94	Na2CO3:H2O
Tobermorite-11A	-23.82	41.57	65.39	Ca5Si6H11O22.5
Tobermorite-14A	-22.08	41.53	63.61	Ca5Si6H21O27.5
Tobermorite-9A	-27.27	41.58	68.86	Ca5Si6H6O20
Todorokite	-0.29	225.78	226.07	Mn7O12:3H2O
Tremolite	-6.96	53.96	60.93	Ca2Mg5Si8O22(OH)2
Tridymite	-0.19	-4.03	-3.84	SiO2
Troilite	-146.86	-184.41	-37.55	FeS
Trona-K	-18.29	-6.70	11.59	K2NaH(CO3)2:2H2O
Tyuyamunite	5.60	9.12	3.52	Ca(UO2)2(VO4)2
U	-204.60	-120.82	83.77	U
U(CO3)2	-59.55	-61.08	-1.53	U(CO3)2
U(g)	-290.15	-120.82	169.33	U
U(HPO4)2:4H2O	-42.18	-84.15	-41.98	U(HPO4)2:4H2O
U(OH)2SO4	-43.97	-56.10	-12.12	U(OH)2SO4
U(SO3)2	-117.59	-156.17	-38.58	U(SO3)2
U(SO4)2	-53.18	-73.76	-20.58	U(SO4)2
U(SO4)2:4H2O	-53.19	-73.79	-20.60	U(SO4)2:4H2O
U(SO4)2:8H2O	-52.20	-73.81	-21.62	U(SO4)2:8H2O
U2C3	-591.67	-522.84	68.84	U2C3
U2Cl10(g)	-226.90	-147.27	79.64	U2Cl10
U2Cl8(g)	-230.32	-166.14	64.17	U2Cl8
U2F10(g)	-243.88	-259.31	-15.44	U2F10
U2F9	-201.36	-257.55	-56.19	U2F9
U2O2Cl5	-120.71	-112.05	8.66	U2O2Cl5
U2O3F6	-126.11	-128.64	-2.53	U2O3F6
U2S3	-571.43	-665.47	-94.04	U2S3
U2Se3	-448.59	-674.02	-225.43	U2Se3
U3As4	-911.92	-924.78	-12.86	U3As4
U3O5F8	-167.72	-170.60	-2.88	U3O5F8
U3P4	-1070.70	-865.89	204.81	U3P4
U3S5	-891.49	-1068.85	-177.36	U3S5
U3Se4	-661.55	-938.96	-277.41	U3Se4
U3Se5	-691.94	-1083.09	-391.15	U3Se5
U4F17	-379.61	-513.33	-133.72	U4F17
U5O12Cl	-74.06	-100.26	-26.20	U5O12Cl
UAs	-269.22	-261.40	7.82	UAs
UAs2	-372.91	-401.98	-29.06	UAs2
UC	-259.15	-214.55	44.60	UC
UC1.94(alpha)	-328.75	-302.66	26.09	UC1.94
UCl(g)	-245.66	-111.38	134.28	UCl
UCl2(g)	-199.70	-101.95	97.75	UCl2
UCl2F2	-92.84	-105.48	-12.64	UCl2F2
UCl2I2	-134.93	-336.34	-201.41	UCl2I2
UCl3	-105.78	-92.51	13.27	UCl3
UCl3(g)	-151.39	-92.51	58.88	UCl3
UCl3F	-95.47	-94.28	1.19	UCl3F
UCl3I	-114.86	-209.71	-94.84	UCl3I
UCl4	-95.94	-83.07	12.87	UCl4
UCl4(g)	-120.37	-83.07	37.30	UCl4
UCl5	-109.38	-73.63	35.75	UCl5

UCl5(g)	-126.60	-73.63	52.97	UCl5
UCl6	-121.69	-64.20	57.50	UCl6
UCl6(g)	-127.56	-64.20	63.37	UCl6
UClF3	-90.05	-116.69	-26.64	UClF3
UClI3	-155.18	-462.98	-307.80	UClI3
UF(g)	-241.34	-122.59	118.76	UF
UF2(g)	-210.68	-124.36	86.32	UF2
UF3	-106.96	-126.12	-19.17	UF3
UF3(g)	-173.61	-126.12	47.49	UF3
UF4	-89.58	-127.89	-38.31	UF4
UF4(g)	-133.37	-127.89	5.48	UF4
UF4:2.5H2O	-85.41	-127.91	-42.49	UF4:2.5H2O
UF5(alpha)	-115.23	-129.66	-14.42	UF5
UF5(beta)	-114.91	-129.66	-14.75	UF5
UF5(g)	-134.46	-129.66	4.80	UF5
UF6	-148.73	-131.42	17.31	UF6
UF6(g)	-149.57	-131.42	18.15	UF6
UH3(beta)	-253.71	-182.63	71.07	UH3
UI(g)	-270.00	-238.02	31.98	UI
UI2(g)	-241.06	-355.22	-114.15	UI2
UI3	-167.71	-472.41	-304.71	UI3
UI3(g)	-214.31	-472.41	-258.11	UI3
UI4	-174.52	-589.61	-415.09	UI4
UI4(g)	-199.53	-589.61	-390.09	UI4
UN	-167.02	-234.94	-67.93	UN
UN1.59(alpha)	-159.46	-302.27	-142.81	UN1.59
UN1.73(alpha)	-157.98	-318.25	-160.27	UN1.73
UO(g)	-205.27	-79.62	125.65	UO
UO2(am)	-29.48	-38.42	-8.94	UO2
UO2(AsO3)2	-79.28	-72.37	6.91	UO2(AsO3)2
UO2(g)	-121.02	-38.42	82.60	UO2
UO2(IO3)2	-18.31	-25.61	-7.29	UO2(IO3)2
UO2(NO3)2	-31.40	-19.45	11.95	UO2(NO3)2
UO2(NO3)2:2H2O	-24.37	-19.46	4.91	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-23.15	-19.47	3.68	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-21.78	-19.49	2.29	UO2(NO3)2:6H2O
UO2(NO3)2:H2O	-27.96	-19.46	8.50	UO2(NO3)2:H2O
UO2(OH)2(beta)	-2.17	2.78	4.95	UO2(OH)2
UO2(PO3)2	-26.58	-42.92	-16.34	UO2(PO3)2
UO2.25	-18.02	-28.12	-10.10	UO2.25
UO2.25(beta)	-18.09	-28.12	-10.02	UO2.25
UO2.3333(beta)	-32.22	-49.37	-17.15	(UO2.3333)2
UO2.6667	-17.53	-21.90	-4.37	(UO2.6667)2
UO2Cl	-26.97	-28.98	-2.02	UO2Cl
UO2Cl2	-31.65	-19.54	12.11	UO2Cl2
UO2Cl2(g)	-67.48	-19.54	47.93	UO2Cl2
UO2Cl2:3H2O	-25.17	-19.56	5.61	UO2Cl2:3H2O
UO2Cl2:H2O	-27.83	-19.55	8.28	UO2Cl2:H2O
UO2ClOH:2H2O	-10.70	-8.40	2.30	UO2ClOH:2H2O
UO2CO3	-4.42	-8.55	-4.13	UO2CO3
UO2F2	-34.69	-41.95	-7.27	UO2F2

UO2F2(g)	-76.58	-41.95	34.63	UO2F2
UO2F2:3H2O	-34.59	-41.97	-7.38	UO2F2:3H2O
UO2FOH	-17.74	-19.59	-1.85	UO2FOH
UO2FOH:2H2O	-16.93	-19.60	-2.67	UO2FOH:2H2O
UO2FOH:H2O	-17.31	-19.60	-2.29	UO2FOH:H2O
UO2HPO4	-7.39	-20.07	-12.68	UO2HPO4
UO2HPO4:4H2O	-7.07	-20.10	-13.03	UO2HPO4:4H2O
UO2SO3	-43.72	-56.09	-12.37	UO2SO3
UO2SO4	-16.82	-14.89	1.93	UO2SO4
UO2SO4:2.5H2O	-13.40	-14.91	-1.50	UO2SO4:2.5H2O
UO2SO4:3.5H2O	-13.42	-14.91	-1.49	UO2SO4:3.5H2O
UO2SO4:3H2O	-13.50	-14.91	-1.41	UO2SO4:3H2O
UO2SO4:H2O	-8.83	-14.90	-6.07	UO2SO4:H2O
UO3(alpha)	-5.86	2.78	8.64	UO3
UO3(beta)	-5.53	2.78	8.31	UO3
UO3(g)	-68.17	2.78	70.95	UO3
UO3(gamma)	-4.93	2.78	7.71	UO3
UO3:.9H2O(alpha)	-2.24	2.78	5.02	UO3:.9H2O
UO3:2H2O	-2.07	2.77	4.84	UO3:2H2O
UOCl	-80.85	-70.18	10.67	UOCl
UOCl2	-57.12	-60.75	-3.63	UOCl2
UOCl3	-62.41	-51.31	11.10	UOCl3
UOF2	-55.95	-83.15	-27.20	UOF2
UOF2:H2O	-55.40	-83.16	-27.76	UOF2:H2O
UOF4	-91.25	-86.69	4.56	UOF4
UOF4(g)	-110.90	-86.69	24.21	UOF4
UOFOH	-42.81	-60.79	-17.98	UOFOH
UOFOH:.5H2O	-42.36	-60.79	-18.43	UOFOH:.5H2O
UP	-308.44	-246.68	61.76	UP
UP2	-453.82	-372.53	81.29	UP2
UP2O7	-42.00	-84.12	-42.12	UP2O7
UP2O7:20H2O	-46.57	-84.25	-37.68	UP2O7:20H2O
UPO5	-19.58	-40.67	-21.09	UPO5
Uraninite	-24.54	-38.42	-13.88	UO2
Uranium-selenide	-211.29	-264.95	-53.65	USe
Uranocircite	-12.66	-32.48	-19.82	Ba(UO2)2(PO4)2
Uranophane	-6.63	10.65	17.29	Ca(UO2)2(SiO3)2(OH)2
US	-253.83	-262.10	-8.27	US
US1.9	-315.71	-389.25	-73.53	US1.9
US2	-324.55	-403.37	-78.83	US2
US3	-426.84	-544.65	-117.81	US3
USe2(alpha)	-240.19	-409.07	-168.88	USe2
USe2(beta)	-240.04	-409.07	-169.03	USe2
USe3	-291.14	-553.20	-262.05	USe3
V	-127.54	-107.80	19.74	V
V2O4	-25.53	-50.80	-25.27	V2O4
V3O5	-68.49	-117.40	-48.91	V3O5
V4O7	-82.35	-142.80	-60.45	V4O7
Vivianite	-46.83	-51.55	-4.72	Fe3(PO4)2:8H2O
Wairakite	-6.10	11.82	17.92	CaAl2Si4O10(OH)4
Weeksite	-25.38	-10.01	15.38	K2(UO2)2(Si2O5)3:4H2O
Whitlockite	-1.92	-6.24	-4.32	Ca3(PO4)2

Witherite	-0.65	-3.67	-3.02	BaCO3
Wollastonite	-4.60	9.13	13.72	CaSiO3
Wurtzite	-128.40	-171.28	-42.88	ZnS
Wustite	-13.43	0.35	13.78	Fe.947O
Xonotlite	-36.99	54.75	91.74	Ca6Si6O17(OH)2
Yb	-154.73	-42.60	112.13	Yb
Yb(OH)3	4.51	19.19	14.69	Yb(OH)3
Yb(OH)3(am)	0.21	19.19	18.99	Yb(OH)3
Yb2(CO3)3	6.73	4.42	-2.31	Yb2(CO3)3
Yb2O3	-9.39	38.41	47.80	Yb2O3
YbF3:.5H2O	-31.90	-47.90	-16.00	YbF3:.5H2O
YbPO4:10H2O	8.07	-3.71	-11.78	YbPO4:10H2O
Zincite	0.00	11.20	11.20	ZnO
Zn	-55.79	-30.00	25.79	Zn
Zn(BO2)2	1.59	9.90	8.31	Zn(BO2)2
Zn(ClO4)2:6H2O	-62.62	318.45	381.06	Zn(ClO4)2:6H2O
Zn(g)	-72.41	-30.00	42.41	Zn
Zn(IO3)2	-11.87	-17.19	-5.32	Zn(IO3)2
Zn(NO3)2:6H2O	-14.47	-11.07	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-0.74	11.19	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-0.47	11.19	11.66	Zn(OH)2
Zn(OH)2(gamma)	-0.69	11.19	11.88	Zn(OH)2
Zn2(OH)3Cl	-4.07	11.23	15.29	Zn2(OH)3Cl
Zn2SiO4	4.53	18.37	13.84	Zn2SiO4
Zn2SO4(OH)2	-2.86	4.72	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-50.86	-41.55	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-20.84	-1.75	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-8.93	33.74	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.20	-11.13	7.08	ZnCl2
ZnCl2(NH3)2	-136.14	-362.99	-226.85	ZnCl2(NH3)2
ZnCl2(NH3)4	-268.45	-714.85	-446.40	ZnCl2(NH3)4
ZnCl2(NH3)6	-402.44	-1066.71	-664.28	ZnCl2(NH3)6
ZnCO3:H2O	-0.28	-0.14	0.14	ZnCO3:H2O
ZnF2	-33.04	-33.54	-0.49	ZnF2
ZnI2	-49.13	-264.40	-215.27	ZnI2
ZnSeO3:H2O	-14.76	-50.53	-35.77	ZnSeO3:H2O
ZnSO4	-10.01	-6.47	3.53	ZnSO4
ZnSO4:6H2O	-4.81	-6.51	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.64	-6.52	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-5.93	-6.48	-0.55	ZnSO4:H2O
Zoisite	-6.74	36.40	43.14	Ca2Al3(SiO4)3OH

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End of simulation.
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Reading input data for simulation 3.
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End of run.
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