
TECHNICAL MEMORANDUM

TO: ADAM ARGUELLO, P.E., SENIOR HYDROGEOLOGIST, HOMESTAKE MINING COMPANY
FROM: DAVID LEVY, PH.D., SENIOR GEOCHEMIST, WORTHINGTON MILLER ENVIRONMENTAL LLC
SUBJECT: GEOCHEMICAL CONDITIONS AFFECTING COC TRANSPORT IN THE SAN ANDRES/GLORIETA AQUIFER SYSTEM, CIBOLA COUNTY, NEW MEXICO (REVISION 1)
DATE: MAY 18, 2021

1.0 Introduction

Homestake Mining Company (HMC) has requested that Worthington Miller Environmental (WME) evaluate geochemical conditions with respect to transport of constituents of concern (COCs) in the San Andres/Glorieta (SAG) Aquifer System in the vicinity of the HMC Grants Reclamation Project (GRP). Prior investigations have been conducted to characterize geochemical properties affecting COC transport (primarily U, Mo, and Se) in the overlying Alluvial Aquifer (WME, 2020a,b). It was demonstrated that conditions in the Alluvial Aquifer are circum-neutral and oxidizing, such that dissolved U, Mo, and Se mainly occur as negatively-charged oxyanions, and consequently their downgradient transport is primarily controlled by weak adsorption to Fe oxide minerals (mainly ferrihydrite, or Fe(OH)₃) (WME, 2020c). However, little information exists to assess factors controlling COC transport in the underlying SAG Aquifer. The objectives of this investigation were to characterize both the mineralogical and aqueous geochemical properties of the system to develop a conceptual understanding of factors controlling potential COC transport in the SAG Aquifer.

2.0 Transport Assessment Approach

Constituent mobility is controlled by pH and oxidation-reduction (redox) conditions, which determines their dissolved forms in groundwater. The mineralogical composition of the aquifer solids is equally important in assessing potential reactions controlling COC transport in the aquifer. Therefore, the transport assessment approach utilizes complete water quality analyses and mineralogical characterization of select SAG Aquifer samples to develop a conceptual model for COC transport, particularly U. It was hypothesized that conditions may be more reducing in the SAG Aquifer compared to the overlying, near-surface Alluvial Aquifer. As a consequence, the factors controlling U transport in the SAG Aquifer may be quite different from those in the Alluvial Aquifer. For example, if conditions are adequately reducing, Fe oxides may not be stable and U could precipitate as insoluble U(IV) (uraninite, or UO₂), rather than being controlled by adsorption of U(VI) to Fe minerals in an oxidizing environment. Therefore, a main focus of this investigation was to characterize the groundwater redox conditions in the SAG Aquifer. The geochemical speciation model PHREEQC (Parkhurst and Appelo, 2013) was further utilized to predict the dominant forms of dissolved COCs and potential for precipitation and/or adsorption which may act to control their concentrations upon migration into the SAG Aquifer.

3.0 Sample Collection and Analysis

The data for this assessment were collected as a component of the geotechnical investigation conducted by HDR (HDR, 2021). Two borings (SAG-1 and SAG-2) were advanced into the Glorieta Sandstone (GSS) with monitoring wells completed in both the GSS and the San Andres Limestone (SALS). Aquifer solids (two sample each from the GSS and SALS) were collected for bulk mineral identification using X-ray diffraction analysis (XRD) and for examination of both major and minor minerals using optical mineralogy (DCM Science Laboratory, Lakewood, CO). The samples were also analyzed for total/inorganic carbon and sulfur content (ACZ Laboratories, Steamboat Springs, CO) which provides an overall indication of inorganic carbonate, detrital organic matter, and/or sulfide mineral content (e.g. pyrite) to assess the reduction capacity of the aquifer solids. Complete lithologic descriptions and all original mineralogical and analytical laboratory reports are included as attachments to the HDR (2021) report.

Groundwater samples were collected from Wells SAG-1 and SAG-2 in February and April of 2021 using sampling methodology proposed by the Water FLUTE system designers in conjunction with a flow cell to obtain representative samples. Five samples were collected from each well at various depths. Field parameters included temperature, pH, dissolved oxygen (DO), electrical conductivity (EC), oxidation-reduction potential (ORP) expressed as Eh, and ferrous iron (Fe as Fe²⁺). All samples were appropriately filtered and/or preserved as required in the field and analyzed for a complete suite of major cations, major anions, nutrients, metals, and radionuclides by ACZ Laboratories, Inc. (Steamboat Springs, CO). Additional samples were also collected from site Wells 0943M and 0951R in March 2021 to provide supplemental information in support of the transport assessment.

4.0 Aquifer Mineralogy and Water Quality Results

Bulk XRD results indicate samples from the SALS consisted primarily of calcite and/or dolomite (97%), with a small amount of quartz (1%) and < 5% unaccounted (Table 1). Samples from the GSS contained much lower carbonate mineral content (6 to 16%) and consisted primarily of quartz (62 to 82%) with lesser amounts of kaolinite and potassium feldspar. Optical microscopy results for these sample were very consistent with respect to major mineral constituents. Microscopy also revealed the presence of minor constituents which could not be detected using XRD. These include pyrite in association with relatively minor Fe oxides in both the SALS and GSS (Table 2).

The carbon and sulfur results were previously reported along with total metal concentrations in HDR (2021). The total carbon contents are mainly comprised of inorganic carbon (carbonate), with only minor organic carbon, and are highest in the SALS samples as would be expected for carbonate rocks. The total sulfur content of the SALS samples consisted of either sulfate-sulfur or sulfide-sulfur (pyrite), while the sulfur content of the GSS is largely dominated by sulfide-sulfur. The presence of organic carbon and pyrite in a number of samples may tend to reflect reducing conditions within the SALS and GSS aquifers, depending of the relative rates of oxygen depletion versus oxygen replenishment from surface recharge.

Groundwater quality results are reported in Table 3 (February 2021) and Table 4 (April 2021) which include sampling depths with elevations, sampling field parameters, and laboratory parameters for the SAG wells sampled. The field QA/QC results indicate all constituents were below detection in the

field blank in February, but that low concentrations of alkalinity and chloride were detected in the field blank in April. For both sampling events, the relative percent difference (RPD) between the primary and duplicate samples were below 20% for all analytes except for the radionuclides, which were detectable at low concentrations and with large ranges in precision. The major ion results indicate that the groundwater is a calcium-sulfate type water (Figure 1) with a tendency toward higher proportions of calcium relative to sodium, and sulfate relative to bicarbonate, with increasing depth in the aquifer. The total dissolved solids (TDS) concentrations ranged from 820 to 1,980 mg/L with the highest TDS concentrations measured at lower depths (Tables 3 and 4). Depth trends for the primary TDS constituents (calcium and sulfate) are shown on Figure 2 where notable increases in both calcium and sulfate occur below a groundwater elevation of 6250 ft amsl. Higher concentrations at depth may be the result of isolation from the effects of dilution by surface recharge and/or longer residence time and water-rock interaction in the deeper groundwater.

A notable observation at both SAG-1 and SAG-2 is the presence of a redox profile, where conditions become more reducing with depth. The shallower samples from SAG-2 tend to have higher DO (Figure 3a) and redox potential (Eh) values (Figure 3b) compared to those samples collected at depth. Ferrous Fe concentrations were also generally higher at depth (Tables 3 and 4) and tend to increase with decreasing redox potential (Figure 4a). The relationships are generally consistent with the expected redox behavior in groundwater (Langmuir, 1997), where measurable ferrous Fe is only present under reducing conditions when DO is low or absent (Figure 4b). Similar trends were observed for nitrogen in the groundwater, where detectable ammonia-N only occurs under reducing conditions when nitrate-N (oxidized form) is low or absent (Figure 5a). Reducing conditions in groundwater can occur when the rate of oxygen consumption exceeds the rate of oxygen replenishment, as driven by the presence of dissolved organic carbon (DOC). A temperate climate groundwater will usually become oxygen-depleted when it contains ≥ 4 mg/L of DOC (Langmuir, 1997). This is consistent with observations from the SAG Aquifer where relatively lower Eh values (≤ 150 mV) occur above a DOC concentration of 4 mg/L (Figure 5b), with resulting DO concentrations ≤ 0.5 mg/L (Figure 3b).

The concentrations of U and Se are also affected by redox conditions in groundwater. For example, the decrease in Se concentrations with increasing depth (Figure 6a) are consistent with precipitation as elemental Se under relatively lower redox potentials (Figure 6b). Uranium displayed more variable trends and less dramatic decreases with depth in comparison (Figure 7a). The Eh-pH limits for the SAG samples (indicated with blue shading on Figure 7b) indicates that insoluble uraninite ($\text{UO}_2(\text{s})$, the reduced form of U) would not be stable, and that U is expected to predominate in the oxidized state [U(VI)] as dissolved complexes with carbonate.

These findings indicate that the SAG Aquifer is generally more reducing as described for the overlying Alluvial Aquifer. The redox classification of the Alluvial Aquifer has been described as Oxic due to the presence of >1 mg/L DO and where Fe oxides are present (WME, 2020c). The redox properties of the SAG groundwater have characteristics of both a Suboxic environment where low DO is measurable in the presence of Fe and Mn oxides, and an Anoxic environment where DO is largely absent in the presence of pyrite and rhodochrosite (MnCO_3) (Langmuir, 1997).

5.0 Geochemical Modeling

The groundwater data were used as input to the geochemical speciation model PHREEQC (Parkhurst and Appelo, 2013) to calculate mineral saturation index values and the forms of U, Mo, and Se present in the groundwater. This information can be used to assess the potential for direct precipitation and/or adsorption of COCs during transport. The saturation index (SI) indicates the potential for a given mineral to precipitate or dissolve. Positive SI values indicate oversaturation with the potential for a mineral to precipitate, while negative SI values indicate undersaturation where the mineral would not precipitate or would be unstable and dissolve if present. By definition, an SI = 0 indicates equilibrium with respect to a given mineral phases, although due to inherent uncertainties in thermodynamic and analytical data, equilibrium with a given mineral phase is generally considered to exist in the range of $-0.50 < SI < +0.50$. The PHREEQC output file shows the preliminary input information followed by all output calculations and is provided as Attachment 1.

The calculate SI values (Table 5) indicate equilibrium or oversaturation with respect to calcite and dolomite, as would be expected based on the mineralogy (Table 1). The majority of the samples were also oversaturated or in near-equilibrium with the Mn(II)- and Fe(II)-bearing carbonate minerals rhodochrosite and siderite, but with a tendency towards undersaturation at higher Eh values (SAG2-1, SAG-2-2, 0951R). The presence of low Fe(III) concentrations also predicts that the groundwaters are oversaturated with respect to ferrihydrite (Table 5) and crystalline Fe oxides such as goethite (not tabulated). Oversaturation with respect to these Fe oxide minerals is consistent with the identification of trace goethite and Fe oxides identified using optical microscopy (Table 2).

In neutral and slightly alkaline environments, powellite (CaMoO_4) is the primary mineral phase with the potential to control Mo concentrations. However the SAG groundwater samples are highly undersaturated with respect to powellite and therefore Mo would not be expected to precipitate in this environment. A number of the samples were near equilibrium or oversaturated with respect to iron selenide (FeSe) and/or amorphous Se, which may act to maintain low Se concentrations in the SAG groundwater, and is consistent with the relationships shown on Figure 6. Measurable U was present in the groundwater samples (Tables 3 and 4), and a high degree of uraninite undersaturation was calculated, indicating that conditions are adequately oxidizing to prevent the precipitation of uraninite.

The solution speciation results for the COCs calculated using PHREEQC were entirely consistent among all samples and therefore not tabulated. The results indicated that virtually 100% of the dissolved Mo exists as the free molybdate ion (MoO_4^{2-}), 100% of the dissolved Se exists as the reduced selenate [Se(IV)] ion (HSeO_3^- and SeO_3^{2-}), and 100% of the dissolved U exists in the form of oxidized U(VI) complexed with calcium and carbonate ($\text{Ca}_2\text{UO}_2(\text{CO}_3)_3^0$ and $\text{CaUO}_2(\text{CO}_3)_3^{2-}$).

6.0 Implications for Uranium Transport in the SAG Aquifer

The pH and Eh conditions in the SAG Aquifer are such that U occurs primarily in its soluble, oxidized form as mobile calcium-carbonate complexes, which are only weakly attenuated by reactive mineral surfaces. The range in pH-Eh conditions measured in the SAG Aquifer as shown on Figure 7 (for the U-CO₃-SO₄ system) indicates the samples fall within the range of stability for oxidized U-carbonate complexes, as supported by geochemical speciation results. Potential adsorbing minerals which have

been identified in the SAG Aquifer include unspecified Fe oxides (likely ferrihydrite) and goethite, a more crystalline form of ferrihydrite (Table 2). Thus, it can be expected that adsorption of U(VI) would be the primary geochemical factor controlling U transport in the SAG Aquifer.

The measured Fe content of the SALS samples ranged from 0.0934 to 0.413% as Fe (HDR, 2021), with an average (N=4) of 0.27% as Fe. For comparison, these values approximate the same range in ferrihydrite estimated from selective chemical extraction of Alluvial Aquifer samples (0.01 to 0.38% as Fe, N=27) (WME, 2020c). Considering this range in alluvial ferrihydrite content, a site-specific surface complexation mixing model (SCCM) was previously utilized to predict the adsorption behavior of COCs in the Alluvial Aquifer. Freundlich adsorption constants for the COCs were subsequently derived using a conservatively low ferrihydrite content of 0.05% as Fe (HMC, 2020) to account for the expected lower adsorption efficiency in the actual groundwater system. Because both the forms of dissolved U and the content of the adsorbing phase (ferrihydrite) in the SAG Aquifer are essentially identical to those of the Alluvial Aquifer, U transport within the SAG Aquifer can also be appropriately and conservatively modeled using the Freundlich parameters previously developed for the Alluvial Aquifer (HMC, 2020).

7.0 References

HDR. 2021. Characterization of the San Andres-Glorieta Aquifer at Homestake Mining Company Superfund Site Near Grants, New Mexico.

Langmuir, D.L. 1997. Aqueous Environmental Chemistry. Prentice Hall, NJ. 600 pp.

Parkhurst, D.L., and Appelo, C.A.J., 2013, Description of input and examples for PHREEQC version 3— A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations: U.S. Geological Survey Techniques and Methods, book 6, chap. A43, 497 p., available only at <http://pubs.usgs.gov/tm/06/a43>

Worthington Miller Environmental LLC (WME). 2020a. Geochemical Characterization of Tailings, Alluvial Solids and Groundwater, Grants Reclamation Project. Prepared for Homestake Mining Company. May.

Worthington Miller Environmental LLC (WME). 2020b. 2019 Supplemental Tailings and Alluvial Characterization Study, Grants Reclamation Project. Prepared for Homestake Mining Company. April.

Worthington Miller Environmental (WME). 2020c. Conceptual Geochemical Model for the Alluvial Aquifer, Grants Reclamation Project. September.

Tables

Table 1. XRD Mineralogy Results (% By Weight) for the SALS and GSS Samples.

Boring	SAG-1	SAG-2	SAG-1	SAG-2
Formation	San Andres LS	San Andres LS	Glorieta SS	Glorieta SS
Lithology	Limestone	Dolostone	Sandstone	Sandstone
Interval (ft)	235.5-236.5	244-245	464-465	439.5-440.5
Sample ID	SAG1-SALS- 235.5-236.5	SAG2-SALS- 244-245	SAG1-GSS- 464-465	SAG2-GSS- 439.5-440.5
ACZ ID	L63831-02	L63799-03	L63831-05	L63799-04
Calcite	79	<2 ¹	6	3
Dolomite	18	97	10	3
Illite	-----	-----	<2 ¹	<2 ¹
Kaolinite	-----	-----	12	4
K-Feldspar	-----	-----	8	6
Quartz	1	1	62	82
Pyrite	-----	-----	-----	<2 ¹
Unaccounted	<5	<5	-----	<5

¹ May be present.

Table 2. Thin Section Optical Mineralogy Results.

Boring	SAG-1	SAG-1
Formation	San Andres LS	Glorieta SS
Lithology	Limestone	Sandstone
Interval (ft)	235.5-236.5	464-465
Sample ID	SAG1-SALS-235.5-236.5	SAG1-GSS-464-465
ACZ ID	L63831-02	L63831-05
Major Mineralogy	<p>Calcite - 81%</p> <p>Dolomite - 18%</p> <p>Quartz - 1%</p>	<p>Quartz - 63%</p> <p>Kaolinite - 12%</p> <p>Dolomite - 10%</p> <p>K-Spar - 8%</p> <p>Calcite - 6%</p> <p>Illite - 6%</p>
Trace Mineralogy	Pyrite, Goethite/Hematite, Mn Oxide, Organic Material	Zircon, Rutile, Apatite, Pyrite, Tourmaline, Iron Oxide, Plagioclase
Petrographic Description	Tan colored limestone primarily containing fine to coarse grained sparry calcite with a grain size that varies from 1 µm to 250 µm. Intermixed with calcite is rhomb shaped grains of dolomite up to 50 µm. Quartz is present in low amounts and occurs as liberated angular fragments and small pockets of fibrous chalcedony up to 275 µm in size. Crosscutting larger fragments of sparry calcite are thin seams of dark brown organic material. The organics commonly carry small pyrite framboids up to 15 µm. Iron oxide is present in trace amounts and occurs as small masses and as pseudomorphs after pyrite. Iron oxide is sometimes seen with black opaque patches of Mn oxide.	Carbonate cemented sandstone primarily containing quartz as angular to well-rounded grains with measurements that vary significantly from 1 µm up to 300 µm. Plagioclase and potassium feldspar are present in low amounts and occur as angular grains up to 150 µm. XRD indicates low levels of clay in the form of kaolinite and illite, however, clay is not discernible in thin section by light microscopy. Dolomite and calcite occur as fine liberated grains in the size range of 1 µm to 75 µm. Pyrite is present as a trace and occurs as liberated fragments and cubes up to 75 µm with no apparent oxidation. Accessory minerals include zircon, honey colored rutile, brown tourmaline, colorless apatite and iron oxide.

Table 3. February 2021 SAG Groundwater Characterization Results.

SAMPLE ID	SAG1-1	SAG1-2	SAG1-3	SAG1-4	SAG1-5	SAG2-1	SAG2-2	SAG2-3	SAG2-4	SAG2-5	0943M	0951R	Field Blank	0999 ¹	RPD
Date	2/22/21	2/23/21	2/23/21	2/25/21	2/25/21	2/26/21	2/26/21	2/26/21	2/26/21	2/26/21	3/23/21	3/23/21	2/25/21	2/26/21	-----
Depth (ft)	260.5	312.5	364.5	394.5	417.5	166.5	207.5	262.5	317.5	372.5	770	470	-----	-----	-----
Elevation (ft amsl)	6299.5	6247.5	6195.5	6165.5	6142.5	6399.5	6358.5	6303.5	6248.5	6193.5	5783.8	6105.8	-----	-----	-----
Dissolved O ₂ (mg/L)	0.15	0.12	0.16	0.11	0.11	2.79	2.2	0.08	0.07	0.14	0.27	0.47	-----	-----	-----
Eh (mV)	25.4	110.2	98.9	51.7	96.0	291.8	326.1	152.5	44.9	84.7	85.8	255	-----	-----	-----
EC (uS/cm)	1238	1390	1488	1817	2011	1220	1216	1228	1234	1351	1930	1822	-----	-----	-----
pH (s.u.)	7.43	7.59	7.63	7.48	7.44	7.21	7.26	7.25	7.56	7.49	7.07	6.98	-----	-----	-----
Temperature (°C)	13.0	13.7	13.8	12.7	12.9	13.1	12.4	12.4	12.9	13.2	15.4	15.2	-----	-----	-----
Calcium (mg/L)	135	144	170	332	402	176	172	176	153	195	201	185	<0.1	175	0.57
Iron (mg/L)	14.9	0.924	1.03	3.46	1.94	<0.06	<0.06	1.2	3.8	2.7	4.25	<0.06	<0.06	<0.06	-----
Fe ²⁺ (mg/L)	3.29	0.89	1.0	2.71	1.84	0.16	0.010	1.0	3.26	2.12	4.6	<0.02	-----	-----	-----
Fe ³⁺ (calc.) (mg/L) ²	11.61	0.03	0.03	0.75	0.10	0.06	0.05	0.20	0.54	0.58	0.06	<0.04	-----	-----	-----
Magnesium (mg/L)	45.5	47.4	50.5	61.3	63.1	46	45.6	46.5	48.2	48.6	62.5	60.6	<0.2	45.7	0.65
Manganese (mg/L)	0.821	4.33	7.61	2.13	3.66	0.046	0.053	0.837	1.91	4.48	0.029	<0.01	<0.01	0.045	2.20
Molybdenum (mg/L)	0.0409	0.0292	0.0351	0.00866	0.0112	0.00211	0.00276	0.0107	0.0175	0.0137	0.00079	0.00181	<0.0002	0.00194	8.40
Potassium (mg/L)	3.99	4.82	4.87	3.64	3.19	4.1	4.01	4.14	4.43	4.13	8.34	8.32	<0.2	4.07	0.73
Selenium (mg/L)	0.00023	0.00021	0.00037	0.0002	0.00018	0.00613	0.00582	0.00364	0.0001	0.00015	0.00782	0.00796	<0.0001	0.0063	2.74
Sodium (mg/L)	95.7	123	123	74.5	72.8	65.3	63.6	67.8	82.8	66.5	172	167	<0.2	64	2.01
Uranium (mg/L)	0.00175	0.00703	0.00537	0.00201	0.00196	0.00705	0.00703	0.0079	0.00486	0.000582	0.00678	0.0255	<0.0001	0.00705	0.00
Vanadium (mg/L)	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	0.00092	<0.0005	<0.0005	-----
Total Alkalinity (mg CaCO ₃ /L)	205	201	174	148	152	261	266	275	237	214	341	317	<2	267	2.27
Bicarbonate Alkalinity (mg CaCO ₃ /L)	205	201	174	148	152	261	266	275	237	214	341	317	<2	267	2.27
Carbonate Alkalinity (mg CaCO ₃ /L)	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	-----
Dissolved Organic Carbon (mg/L)	24.2	9.4	11.8	7.1	12.7	2.2	3.2	32.1	12.5	7.3	<1	<1	<1	1.9	14.6
Chloride (mg/L)	72.6	94.3	91.4	40.3	40	54	55.6	56.7	61.7	55.6	151	141	<0.5	57.3	5.93
Hardness (mg CaCO ₃ /L)	524	555	632	1080	1260	629	617	631	581	687	759	711	<0.2	625	0.64
Nitrate+Nitrite-N (mg/L)	<0.02	<0.02	<0.02	<0.02	<0.02	2.31	2.18	0.025	<0.02	<0.02	3.71	3.78	<0.02	2.35	1.72
Ammonia-N (mg/L)	0.259	0.739	0.579	0.159	0.191	<0.05	<0.05	0.099	0.786	0.216	<0.05	<0.05	<0.05	<0.05	-----
Total Dissolved Solids (mg/L)	860	1120	1140	1670	1960	978	984	970	930	1130	1480	1400	<20	988	1.02
Sulfate (mg/L)	399	461	629	1070	1220	408	410	411	436	593	603	556	<1	411	0.73
Sulfide (mg S/L)	<0.02	<0.02	<0.02	<0.02	0.026	<0.02	<0.02	<0.02	0.026	<0.02	<0.02	<0.02	<0.02	<0.02	-----
Radium-226 (pCi/L)	1 ±0.22	0.17 ±0.24	2.2 ±0.31	0.82 ±0.21	0.44 ±0.19	0.44 ±0.23	0.22 ±0.13	0.3 ±0.17	4.2 ±0.48	1.3	NM	NM	-0.01 ±0.11	0.36 ±0.11	20.0
Radium-228 (pCi/L)	0.33 ±1	0.87 ±0.86	0.62 ±1.1	0.41 ±0.89	-0.2 ±0.84	0.78 ±0.81	0.55 ±0.57	0.44 ±0.99	-0.25 ±0.9	0.67	NM	NM	-0.13 ±0.77	1.4 ±1.1	56.9
Radium-226+228	1.33	1.04	2.82	1.23	0.44	1.22	0.77	0.74	4.2	1.97	NM	NM	-----	1.76	36.2
Thorium-230 (pCi/L)	1.55 ±1.1	0.751 ±2.4	1.34 ±2.1	4.01 ±2.4	4.75 ±3.6	1.01 ±0.59	0.55 ±0.55	3.8 ±3.6	2.55 ±2.4	2.81	NM	NM	1.97 ±1.9	0.183 ±0.26	139

¹ SAG2-1 duplicate. ² Ferric Fe calculated by difference. Bold value indicates a negative value was obtained and the detection limit (0.06 mg/L) was substituted.

Table 4. April 2021 SAG Groundwater Characterization Results.

SAMPLE ID	SAG1-1	SAG1-2	SAG1-3	SAG1-4	SAG1-5	SAG2-1	SAG2-2	SAG2-3	SAG2-4	SAG2-5	Field Blank	0999 ¹	RPD
Date	4/5/21	4/5/21	4/5/21	4/5/21	4/5/21	4/2/21	4/2/21	4/2/21	4/1/21	4/1/21	4/2/21	4/5/21	-----
Depth (ft)	260.5	312.5	364.5	394.5	417.5	166.5	207.5	262.5	317.5	372.5	-----	-----	-----
Elevation (ft amsl)	6299.5	6247.5	6195.5	6165.5	6142.5	6399.5	6358.5	6303.5	6248.5	6193.5	-----	-----	-----
Dissolved O ₂ (mg/L)	0.20	0.19	0.22	0.21	0.19	3.49	2.38	0.53	0.28	0.18	-----	-----	-----
Eh (mV)	29.4	125.4	110.1	77.5	80.6	318.2	308.8	56.7	39.7	56.0	-----	-----	-----
EC (uS/cm)	1389	1405	1543	1879	2119	1256	1250	1221	1265	1556	-----	-----	-----
pH (s.u.)	7.57	7.76	7.65	7.53	7.45	7.35	7.38	7.44	7.75	7.69	-----	-----	-----
Temperature (°C)	14.2	13.9	13.9	13.9	13.2	13.9	13.6	13.7	13.6	13.8	-----	-----	-----
Calcium (mg/L)	131	151	184	345	428	179	177	162	145	236	<0.1	150	0.66
Iron (mg/L)	12.8	0.873	1.02	3.46	1.92	<0.06	<0.06	3.23	4.69	3.04	<0.06	0.858	1.73
Fe ²⁺ (mg/L) ²	4.8	0.95	1.11	2.21	1.91	0.04	0.07	2.97	4.6	2.98	-----	-----	-----
Fe ³⁺ (calc.) (mg/L)	8.00	0.06	0.06	1.25	0.01	0.02	0.06	0.26	0.09	0.06	-----	-----	-----
Magnesium (mg/L)	45.7	49.6	53.1	63.8	65.3	47.2	47.2	46.7	48.4	56.4	<0.2	49	1.22
Manganese (mg/L)	0.738	4.2	6.13	2.01	2.99	0.027	0.03	0.874	2.11	6.5	<0.01	4.14	1.44
Molybdenum (mg/L)	0.02740	0.01940	0.02190	0.00620	0.00806	0.00200	0.00293	0.01000	0.01660	0.01730	<0.0002	0.01930	0.52
Potassium (mg/L)	4.04	4.81	4.89	3.71	2.99	4.17	4.04	4.36	4.32	4.61	<0.2	4.82	-0.21
Selenium (mg/L)	0.00012	<0.0001	0.00013	<0.0001	0.00013	0.00636	0.00567	0.00051	<0.0001	0.00014	<0.0001	<0.0001	-----
Sodium (mg/L)	98.1	122	125	76.7	69.3	66.4	66	70.8	88.8	74.1	<0.2	121	0.82
Uranium (mg/L)	0.00120	0.00662	0.00440	0.00138	0.00143	0.00715	0.00719	0.00623	0.00370	0.00303	<0.0001	0.00669	-1.05
Vanadium (mg/L)	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	-----
Total Alkalinity (mg CaCO ₃ /L)	209	229	180	149	159	295	292	249	250	137	3.6	232	-1.30
Bicarbonate Alkalinity (mg CaCO ₃ /L)	209	229	180	149	159	295	292	249	250	137	3.6	232	-1.30
Carbonate Alkalinity (mg CaCO ₃ /L)	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	-----
Dissolved Organic Carbon (mg/L)	18.3	5.2	6.7	4.5	11.4	1.8	1.5	17.6	10.8	10.6	<1	5.2	0.00
Chloride (mg/L)	72	86.4	88.7	34.9	29.2	53.5	54	56.9	66.2	46	0.68	86.1	0.35
Hardness (mg CaCO ₃ /L)	515	581	678	1120	1340	641	636	597	561	822	<0.2	576	0.86
Nitrate+Nitrite-N (mg/L)	<0.02	<0.02	<0.02	<0.02	<0.02	2.39	2.23	<0.02	<0.02	<0.02	<0.02	<0.02	-----
Ammonia-N (mg/L)	0.281	0.786	0.548	0.109	0.152	<0.05	<0.05	0.379	0.836	0.243	<0.05	0.783	0.38
Total Dissolved Solids (mg/L)	880	1000	1120	1680	1980	980	974	820	840	1180	1.3	980	2.02
Sulfate (mg/L)	446	474	613	1040	1290	394	381	397	426	769	<1	491	-3.52
Sulfide (mg S/L)	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02	0.064	<0.02	<0.02	<0.02	<0.02	-----
Radium-226 (pCi/L)	0.22 ±0.09	0.29 ±0.13	1.1 ±0.17	0.62 ±0.14	0.3 ±0.1	0.36 ±0.13	0.17 ±0.08	0.24 ±0.19	1.3 ±0.25	1.2 ±0.29	0.11 ±0.14	0.17 ±0.07	52.17
Radium-228 (pCi/L)	0.1 ±1.2	0.43 ±1.2	0.47 ±1	-0.73 ±1.2	0.28 ±1.2	0.22 ±0.87	0.28 ±1.1	0.68 ±1.1	0.44 ±1	-0.43 ±0.95	-0.22 ±0.77	-0.51 ±1	-2350
Radium-226+228	0.32	0.72	1.57	0.62	0.58	0.58	0.45	0.92	1.74	1.2	0.11	0.17	124.0
Thorium-230 (pCi/L)	0.407 ±0.3	0.406 ±0.4	0.604 ±0.37	0.208 ±0.32	0.425 ±0.32	0.189 ±0.28	0.393 ±0.31	0.372 ±0.24	0.428 ±0.3	0.424 ±0.26	0.439 ±0.31	0.413 ±0.26	-1.71

¹ SAG1-2 duplicate. ² Ferric Fe calculated by difference. Bold value indicates a negative value was obtained and the detection limit (0.06 mg/L) was substituted.

Table 5. Saturation Index Values Calculated Using PHREEQC.¹

Location	Date	Eh (mV)	Calcite	Dolomite	Rhodochrosite	Siderite	Ferrihydrite	Powellite	Iron Selenide	Selenium	Uraninite
			CaCO ₃	CaMg(CO ₃) ₂	MnCO ₃	FeCO ₃	Fe(OH) ₃	CaMoO ₄	FeSe	Se(am)	UO ₂
SAG1-1	2/22/21	110	0.15	0.01	-0.09	0.05	4.53	-1.48	2.87	4.51	-3.43
SAG1-2	2/23/21	99	0.31	0.35	0.77	-0.38	2.12	-1.63	-7.19	-2.10	-6.20
SAG1-3	2/23/21	52	0.33	0.33	0.96	-0.39	2.16	-1.52	-5.99	-1.30	-5.93
SAG1-4	2/25/21	96	0.30	0.07	0.09	-0.29	3.36	-1.94	-0.36	2.39	-4.40
SAG1-5	2/25/21	292	0.34	0.07	0.27	-0.52	2.46	-1.77	-4.89	-0.45	-5.93
SAG2-1	2/26/21	326	0.14	-0.11	-1.46	-1.38	2.04	-2.66	-22.9	-10.9	-11.7
SAG2-2	2/26/21	153	0.18	-0.04	-1.35	-2.54	1.98	-2.56	-27.9	-13.5	-12.9
SAG2-3	2/26/21	45	0.19	-0.01	-0.15	-0.54	2.57	-1.96	-8.41	-1.95	-7.06
SAG2-4	2/26/21	85	0.38	0.45	0.46	0.22	3.32	-1.81	-0.15	2.16	-4.28
SAG2-5	2/26/21	86	0.34	0.27	0.68	-0.11	3.29	-1.86	-3.89	-0.01	-6.35
0943M	3/23/21	255	0.14	0.00	-1.75	0.01	2.00	-3.13	0.16	3.76	-4.79
0951R	3/23/21	29	-0.01	-0.28	-2.62	-2.46	1.73	-2.79	-18.9	-7.20	-9.52
SAG1-1	4/5/21	125	0.28	0.32	0.01	0.37	4.55	-1.68	1.59	3.21	-4.21
SAG1-2	4/5/21	110	0.55	0.83	0.98	-0.13	2.58	-1.79	-9.80	-4.26	-7.41
SAG1-3	4/5/21	78	0.40	0.46	0.90	-0.31	2.48	-1.69	-7.89	-2.78	-6.65
SAG1-4	4/5/21	81	0.39	0.26	0.13	-0.31	3.69	-2.06	-3.57	0.11	-5.68
SAG1-5	4/5/21	318	0.39	0.16	0.20	-0.48	1.48	-1.90	-3.76	0.23	-5.77
SAG2-1	4/2/21	309	0.35	0.33	-1.50	-1.78	1.73	-2.68	-27.0	-13.5	-13.3
SAG2-2	4/2/21	57	0.37	0.37	-1.43	-1.51	2.22	-2.52	-25.8	-12.9	-12.9
SAG2-3	4/2/21	40	0.32	0.31	0.03	0.11	2.92	-2.02	-0.31	2.52	-4.48
SAG2-4	4/1/21	56	0.57	0.88	0.72	0.60	2.74	-1.86	-0.65	1.40	-4.92
SAG2-5	4/1/21	110	0.40	0.38	0.82	0.01	2.51	-1.71	-1.66	1.04	-4.71

¹ Shaded cells indicate equilibrium or oversaturation with respect to the mineral phase.

Figures

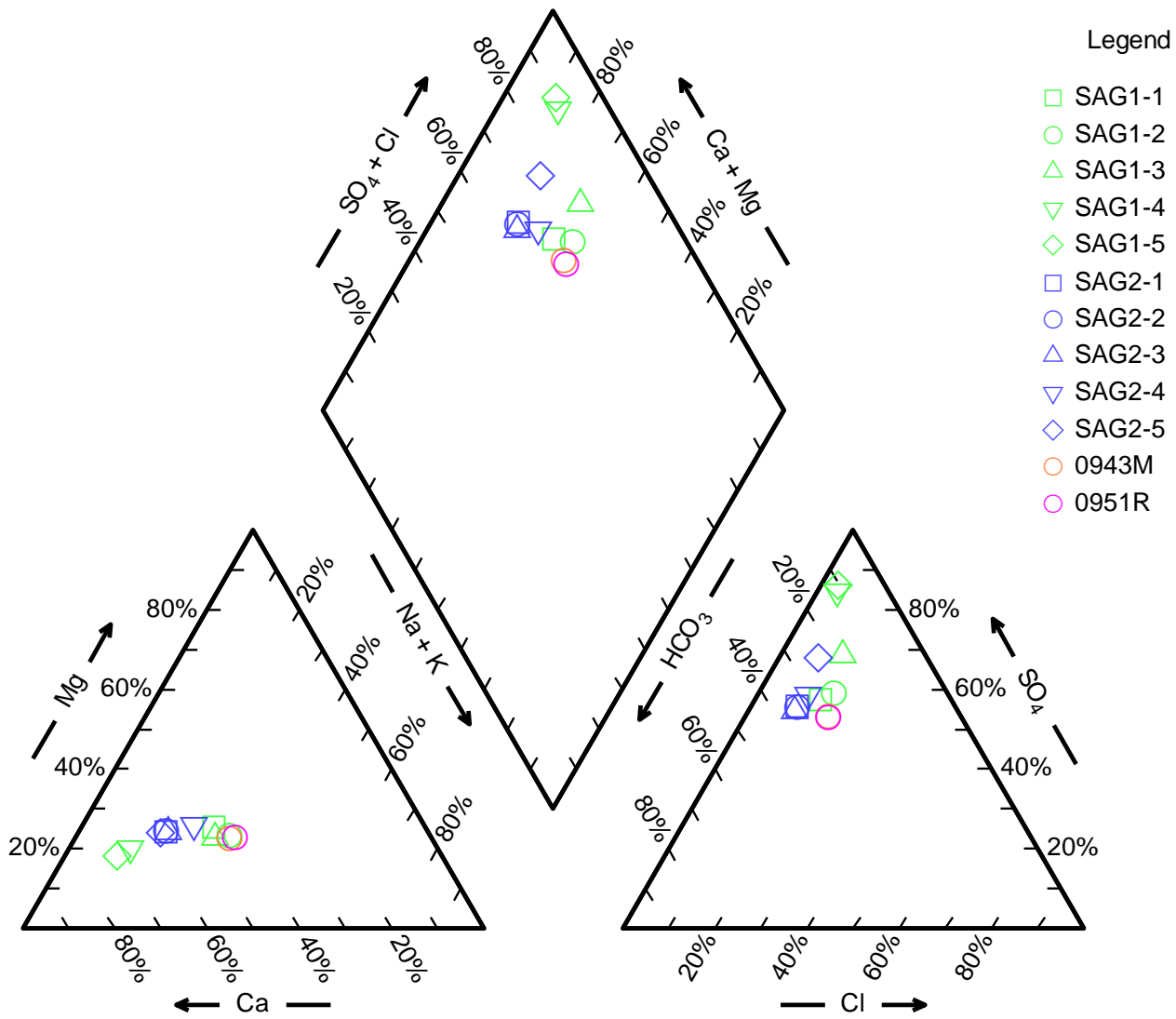


Figure 1: Trilinear Diagram for the Wells Sampled (Only February 2021 Samples Shown for Clarity).

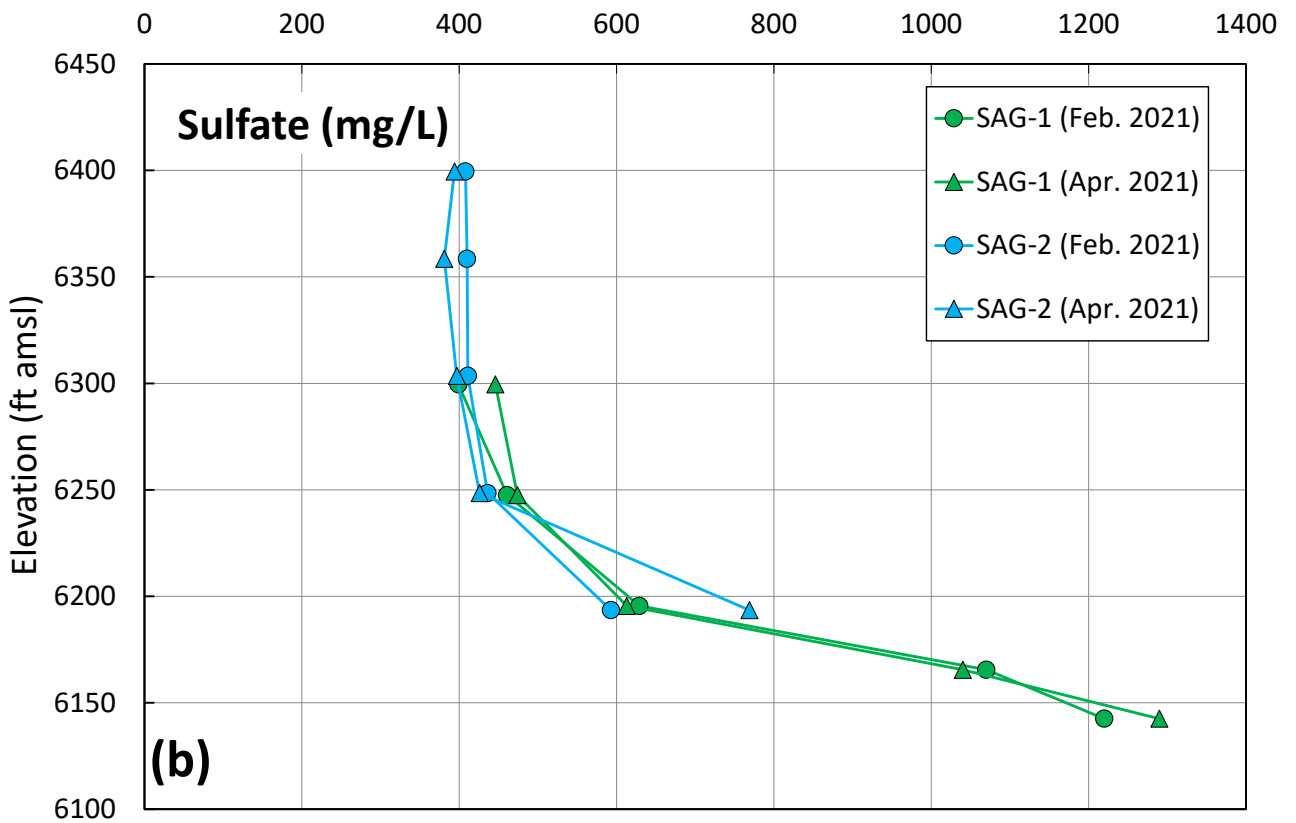
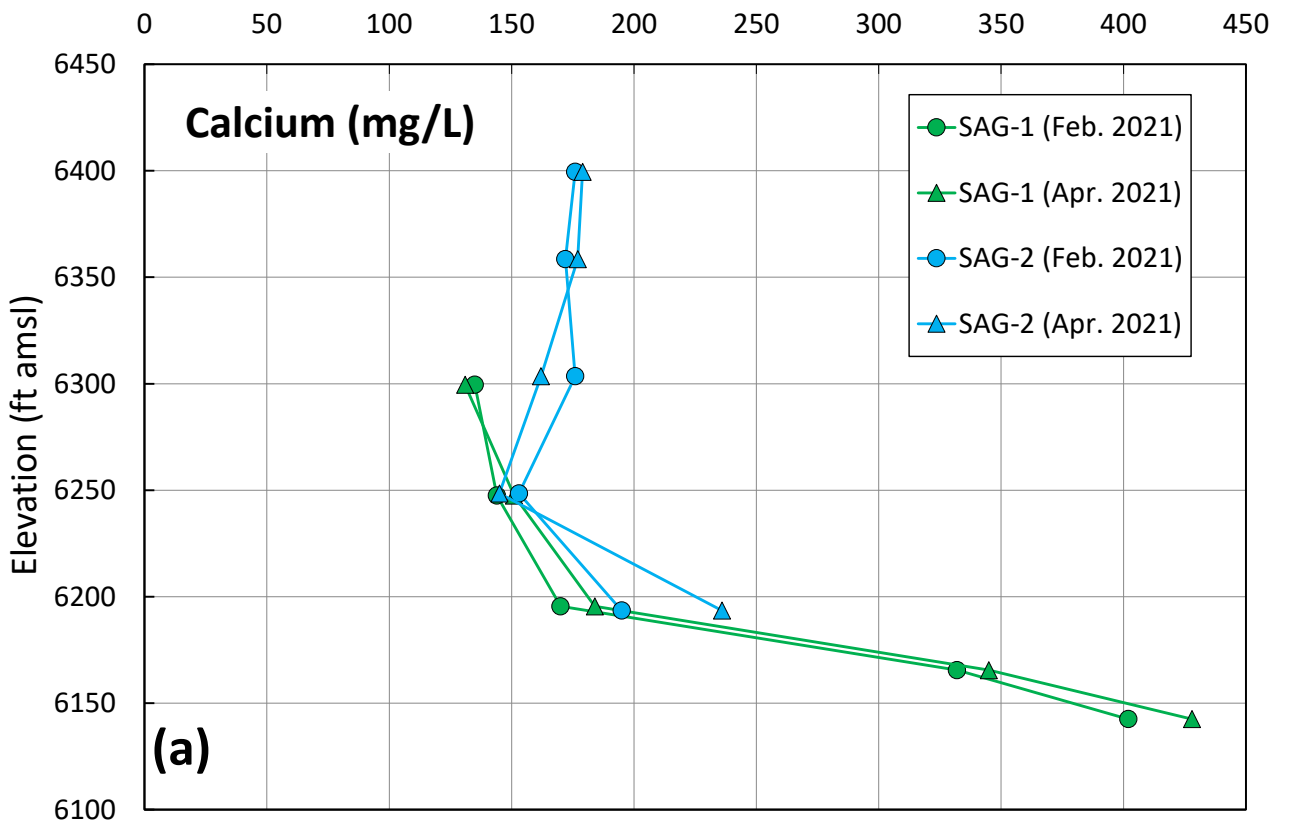


Figure 2: Trends in (a) Calcium and (b) Sulfate With Depth at SAG-1 and SAG-2.

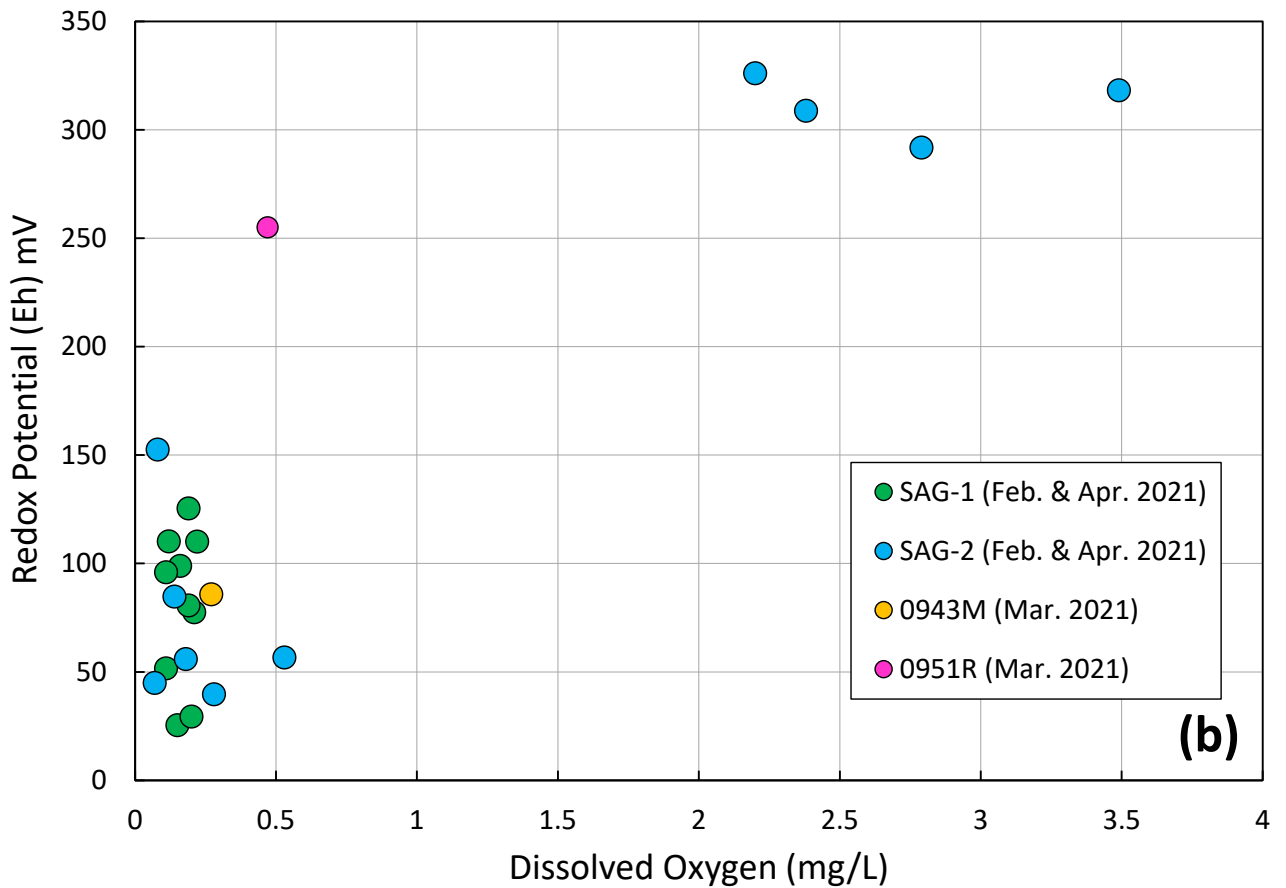
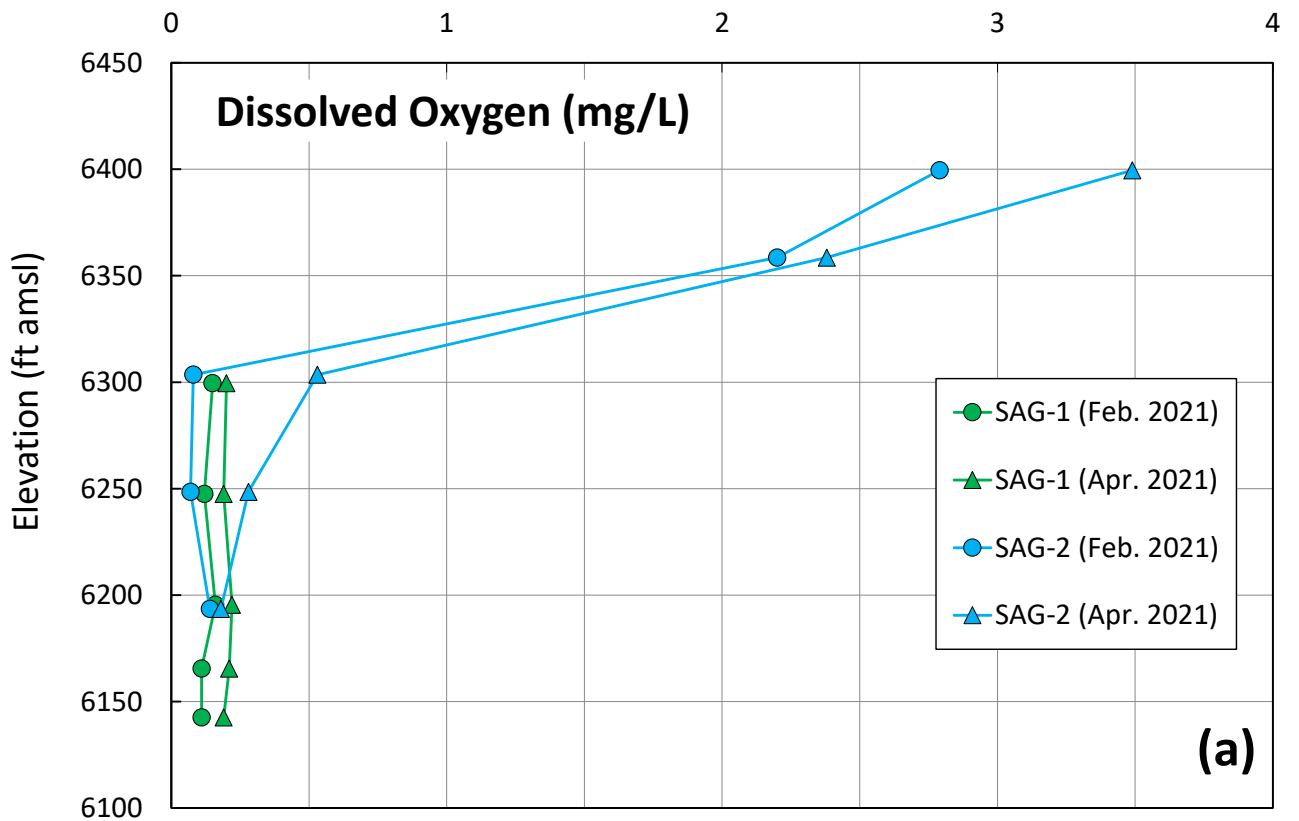


Figure 3: Dissolved Oxygen With Depth (a) and as Related to Redox Potential (b) .

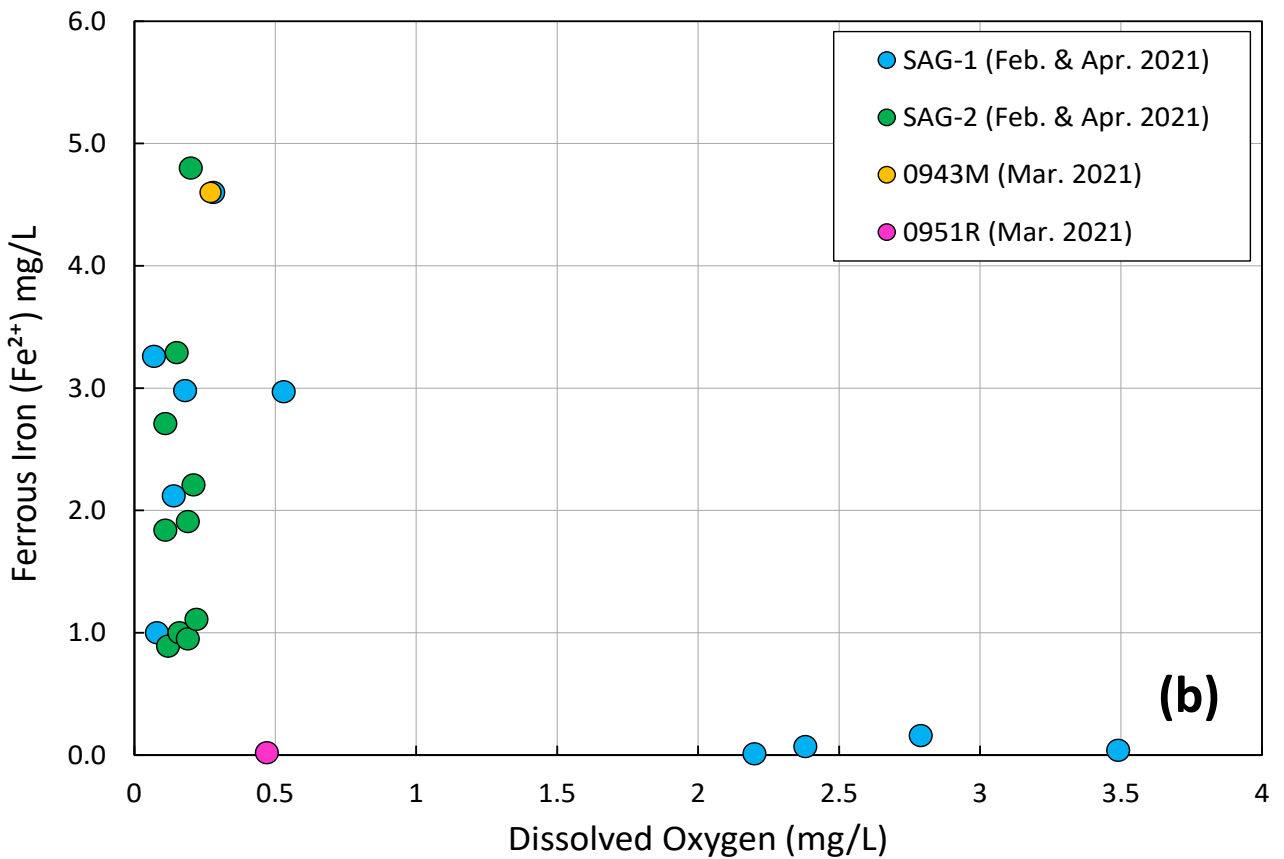
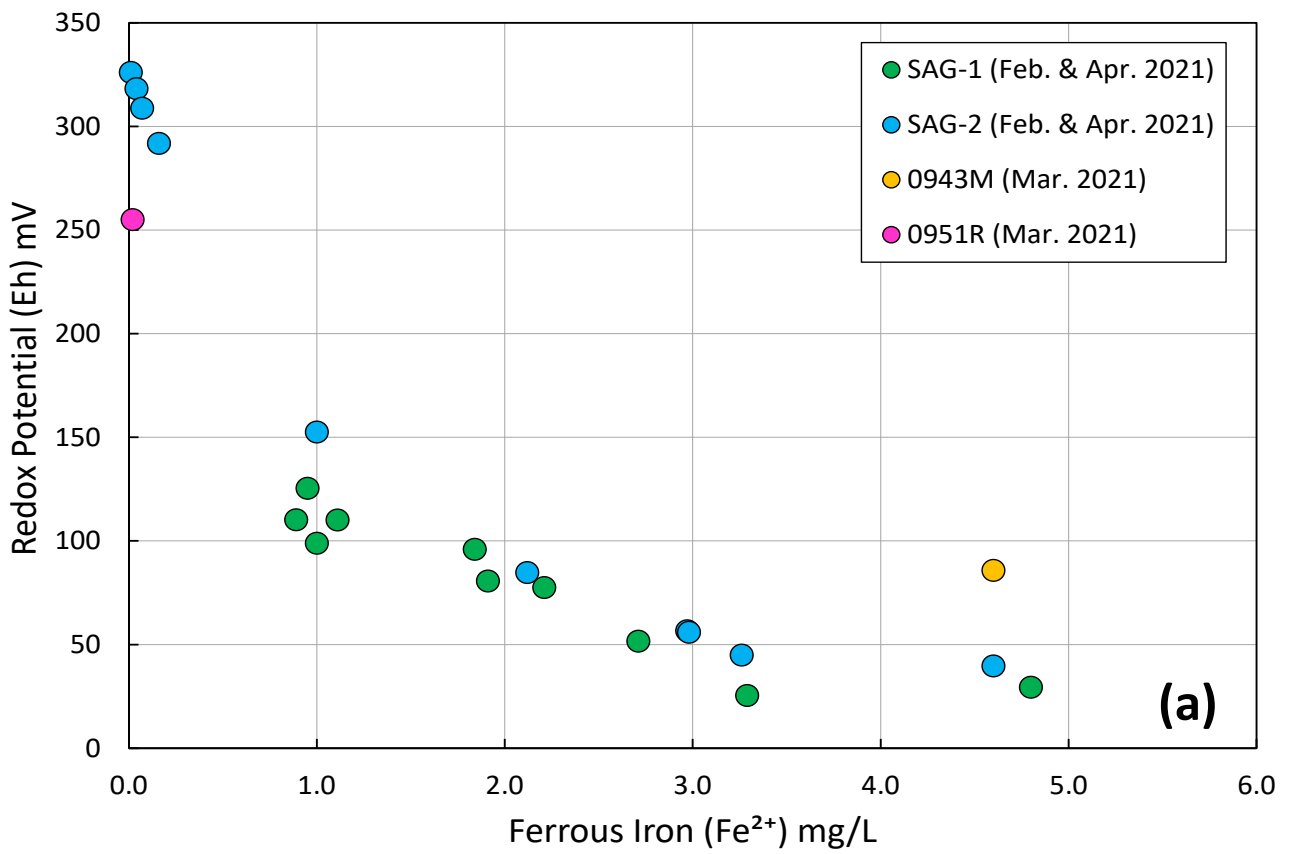


Figure 4: Ferrous Iron as Related to Redox Potential (Eh) (a) and Dissolved Oxygen (b).

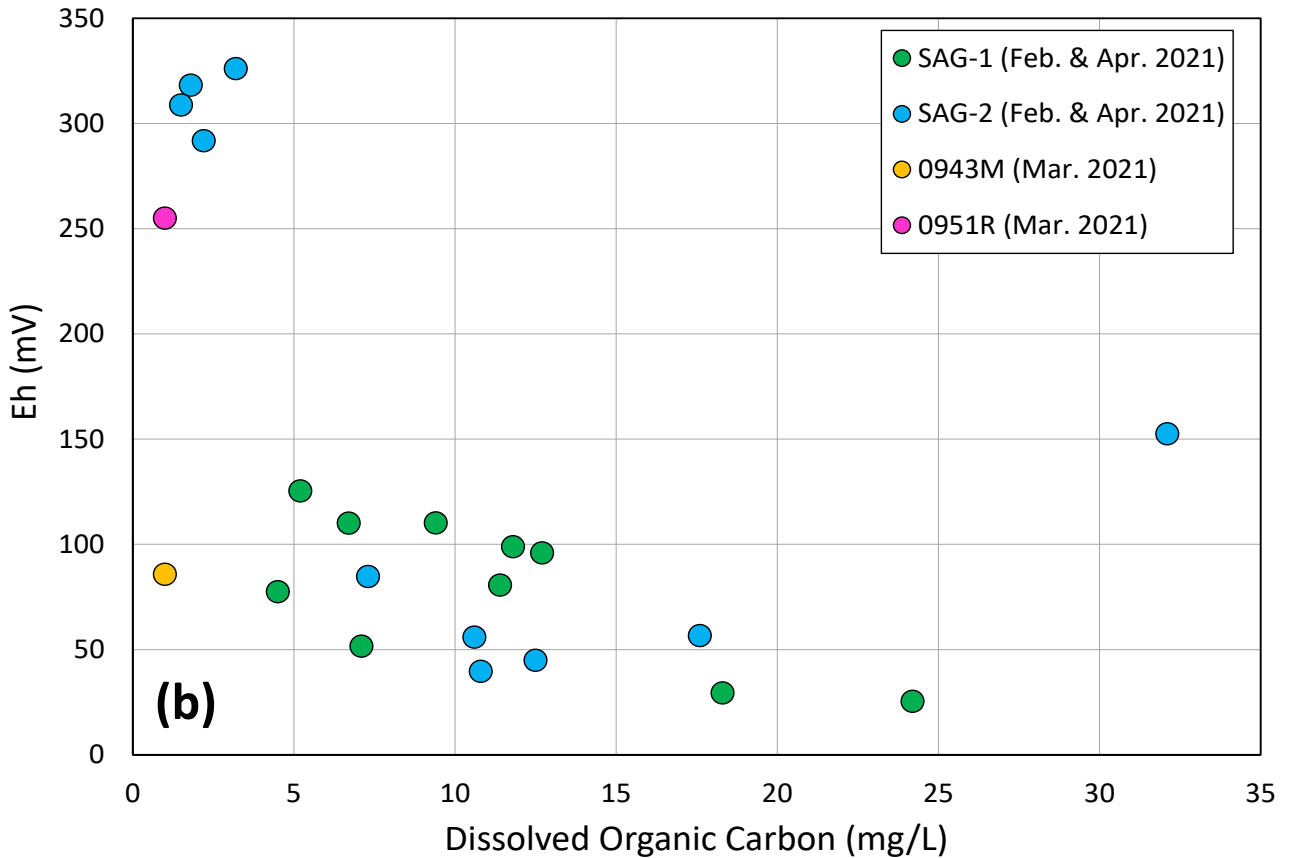
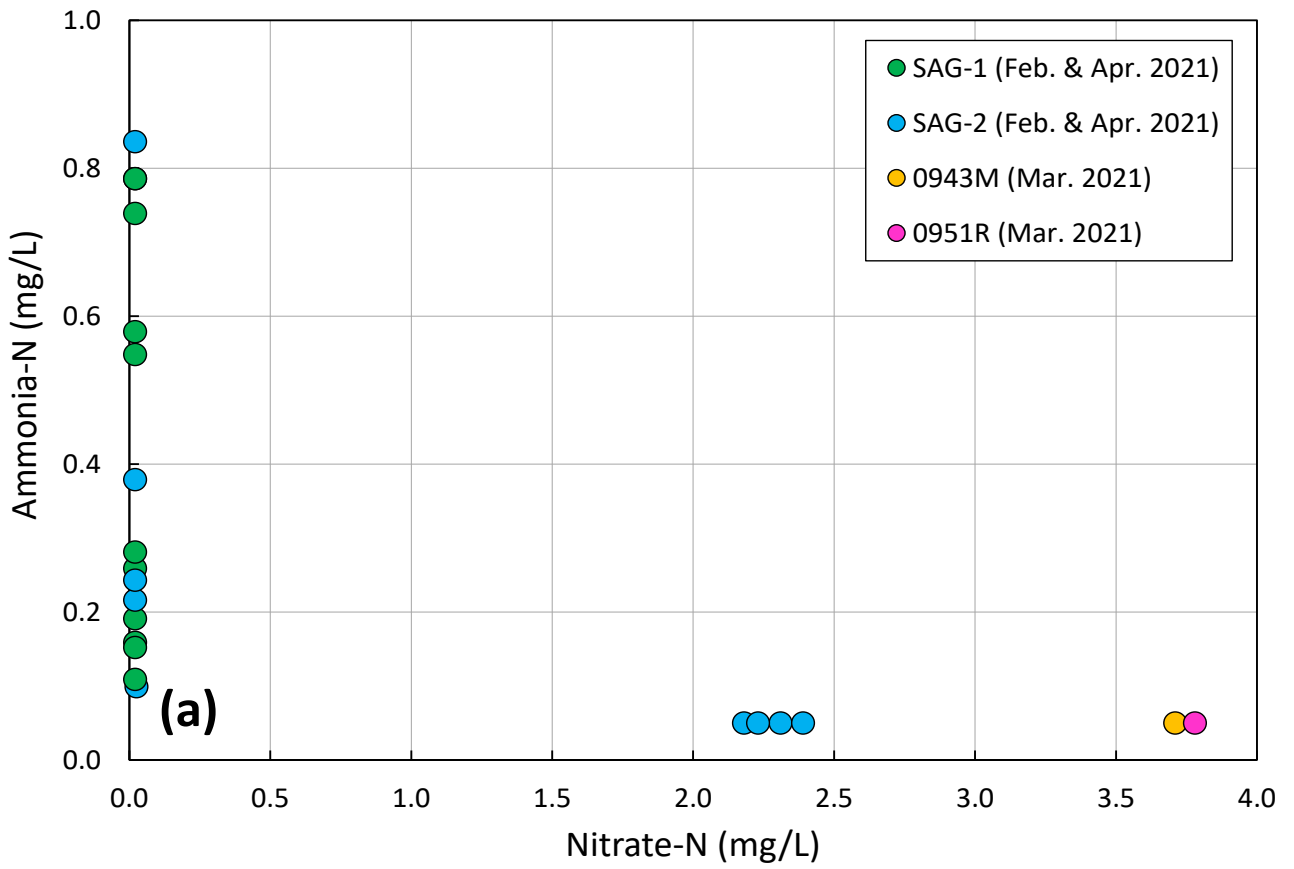


Figure 5: (a) Relationship Between $\text{NH}_3\text{-N}$ and $\text{NO}_3\text{-N}$ and (b) Redox Potential (Eh) as a Function of Dissolved Organic Carbon.

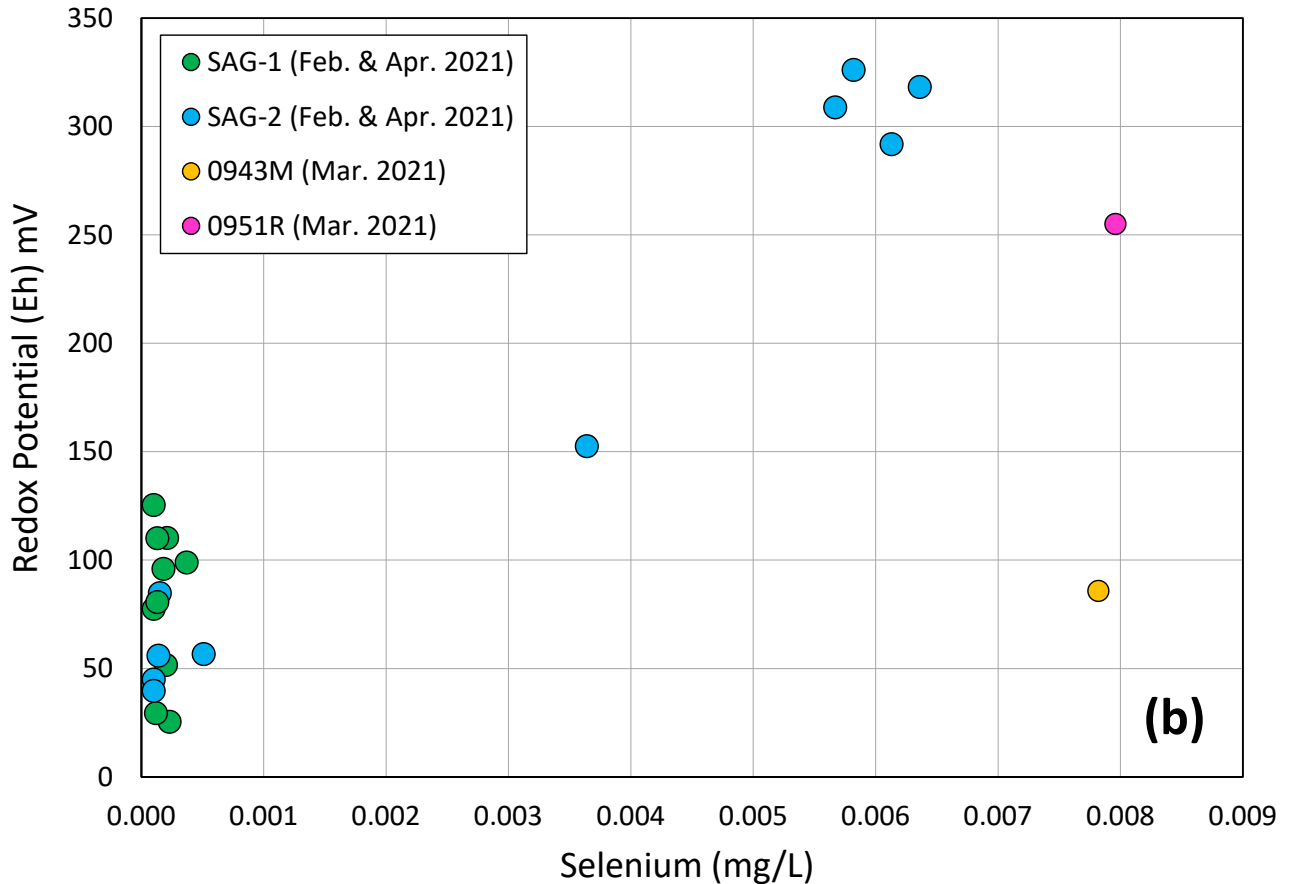
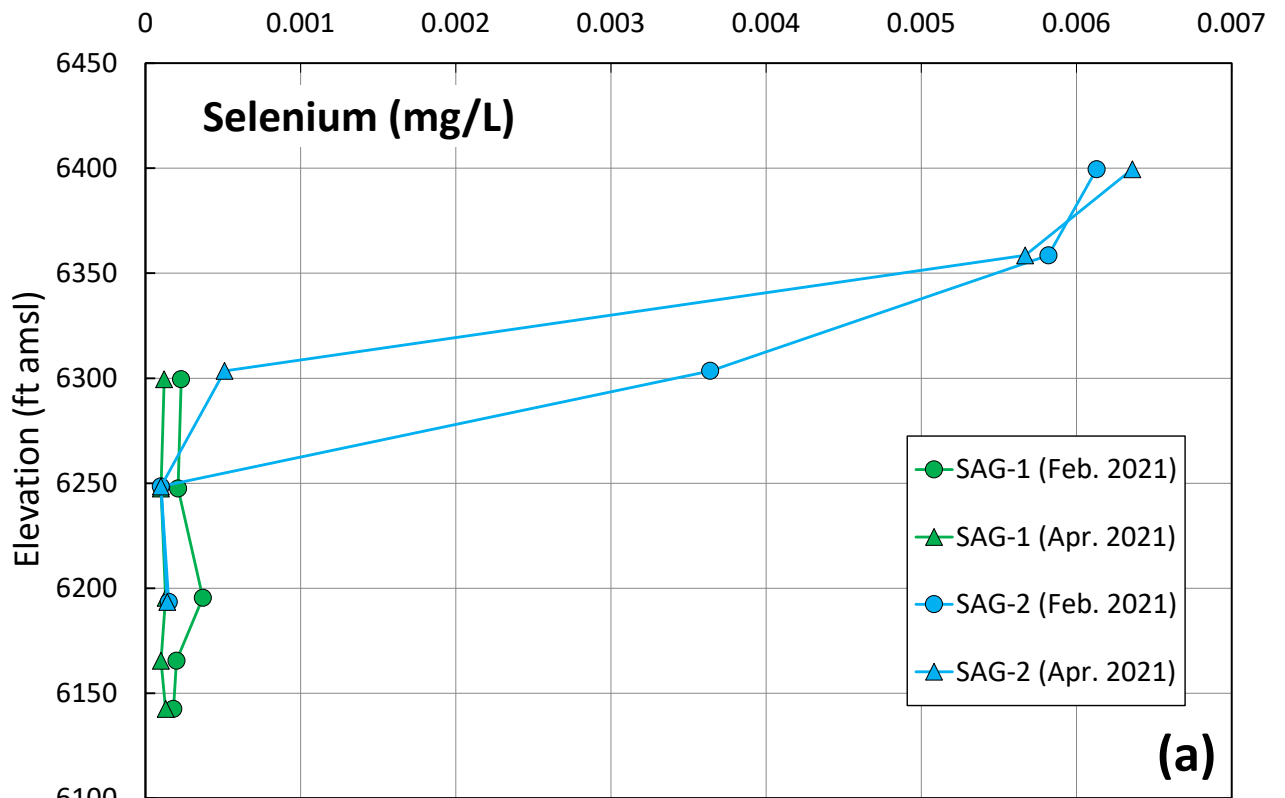


Figure 6: Selenium Concentrations as a Function of Depth (a) and Redox Potential (Eh) (b) .

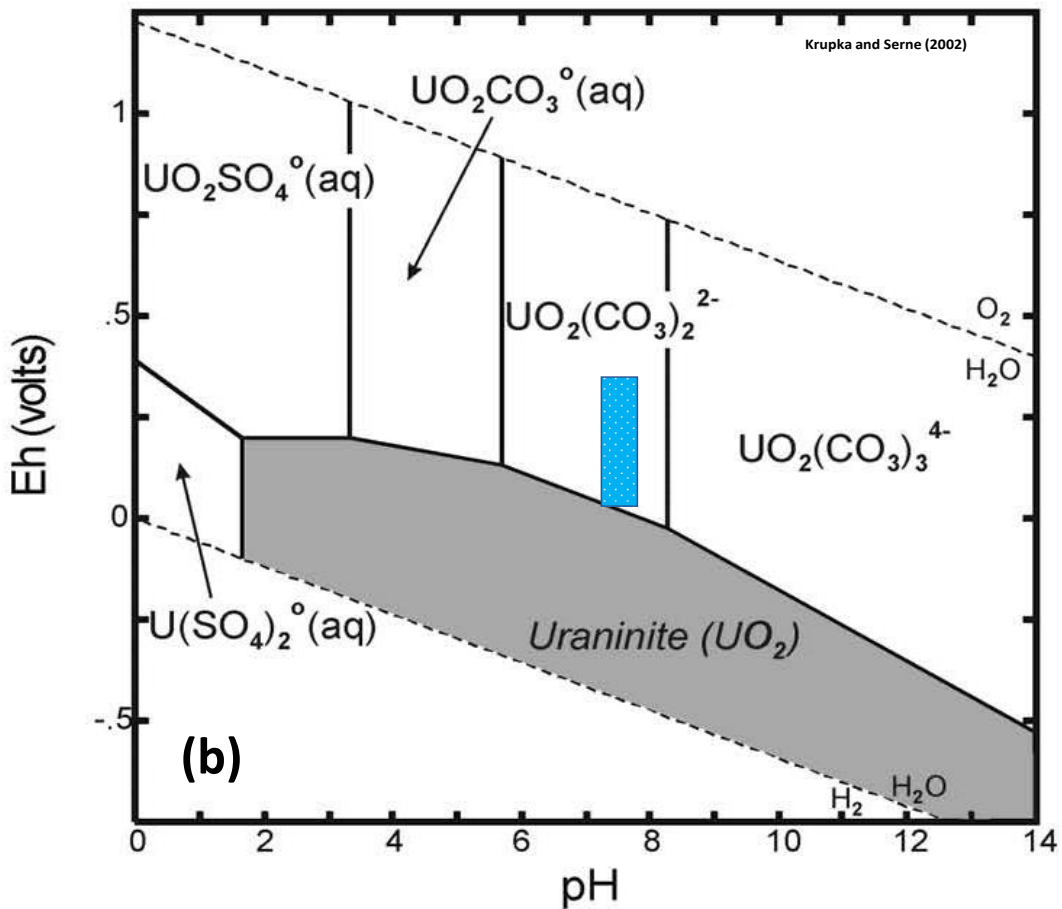
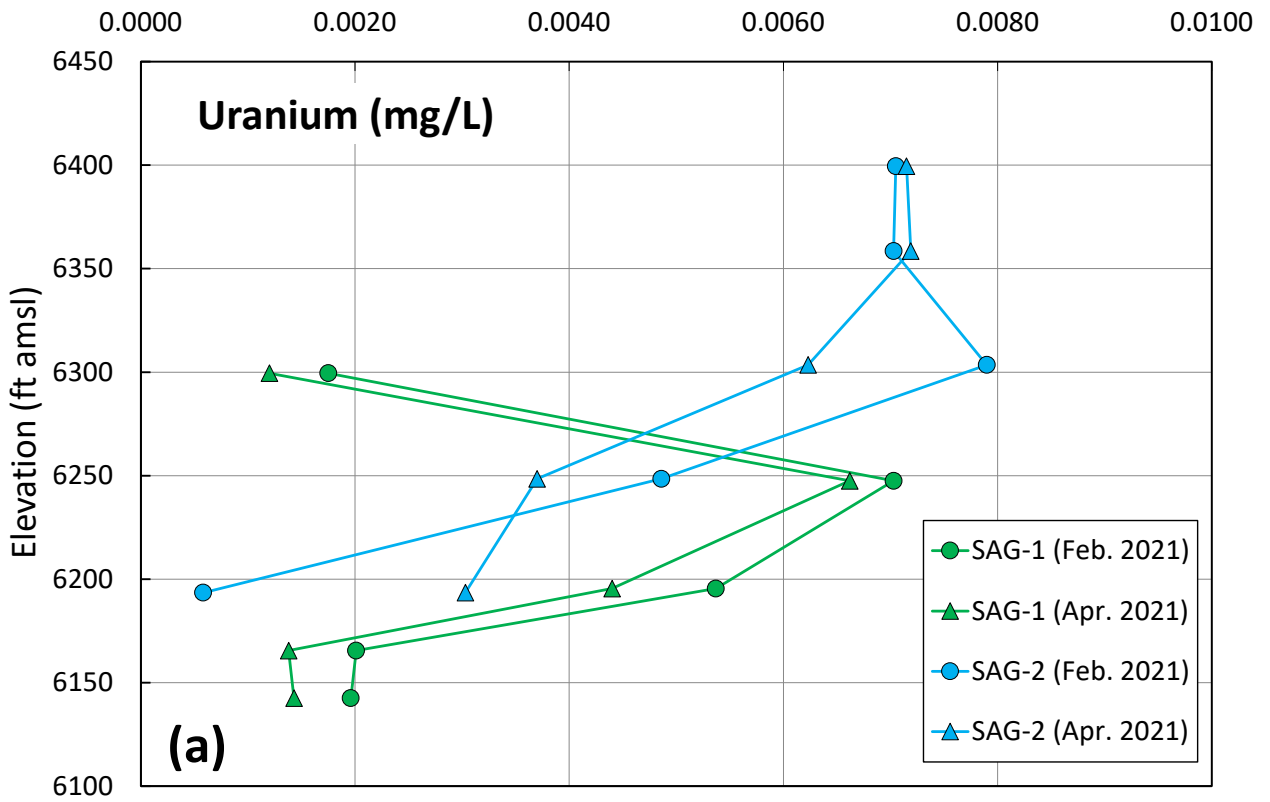


Figure 7: (a) Uranium Concentrations vs. Depth and (b) Stability Diagram for the U-CO₃-SO₄ System (Range of Measured Eh and pH Depicted by the Blue Box).

Attachment 1 - PHREEQC Output File

Input file: C:\Users\dlevy\Desktop\ARCHIVED_PHREEQC\Homestake_SAG_Speciation_2021.pqi
 Output file: C:\Users\dlevy\Desktop\ARCHIVED_PHREEQC\Homestake_SAG_Speciation_2021.pqo
 Database file: C:\Users\dlevy\Desktop\ARCHIVED_PHREEQC\database\Modified_Minteqv4.dat

 Reading data base.

SOLUTION_MASTER_SPECIES
 SOLUTION_SPECIES
 SOLUTION_SPECIES
 PHASES
 PHASES
 SURFACE_MASTER_SPECIES
 SURFACE_SPECIES
 EXCHANGE_MASTER_SPECIES
 EXCHANGE_SPECIES
 END

 Reading input data for simulation 1.

DATABASE C:\Users\dlevy\Desktop\ARCHIVED_PHREEQC\database\Modified_Minteqv4.dat

SOLUTION_SPREAD

Number	Description	pe	Alkalinity	pH	O(0)	Temp	Ca	Fe(2)	Fe(3)	Mg	Mn	
Mo	K	Se	Na	U	Cl	N(5)	N(-3)	S(6)	S(-2)			
units	mg/L											
			as Ca0.5(CO3)0.5									
1	SAG1-1	0.4	205	7.43	0.15	13	135	3.3	11.6	45.5	0.821	0.0409
3.99	0.00023	95.7	0.00175	72.6	0.02	0.259	399	0				
2	SAG1-2	1.9	201	7.59	0.12	13.7	144	0.89	0.03	47.4	4.33	0.0292
4.82	0.00021	123	0.00703	94.3	0.02	0.739	461	0				
3	SAG1-3	1.7	174	7.63	0.16	13.8	170	1.00	0.03	50.5	7.61	0.0351
4.87	0.00037	123	0.00537	91.4	0.02	0.579	629	0				
4	SAG1-4	0.9	148	7.48	0.11	12.7	332	2.71	0.75	61.3	2.13	0.00866
3.64	0.0002	74.5	0.00201	40.3	0.02	0.159	1070	0				
5	SAG1-5	1.6	152	7.44	0.11	12.9	402	1.84	0.10	63.1	3.66	0.0112
3.19	0.00018	72.8	0.00196	40.0	0.02	0.191	1220	0.026				
6	SAG2-1	4.9	261	7.21	2.79	13.1	176	0.16	0.06	46	0.046	0.00211
4.1	0.00613	65.3	0.00705	54.0	2.31	0.05	408	0				
7	SAG2-2	5.5	266	7.26	2.2	12.4	172	0.01	0.05	45.6	0.053	0.00276
4.01	0.00582	63.6	0.00703	55.6	2.18	0.05	410	0				
8	SAG2-3	2.6	275	7.25	0.08	12.4	176	1.00	0.20	46.5	0.837	0.0107
4.14	0.00364	67.8	0.0079	56.7	0.025	0.099	411	0				
9	SAG2-4	0.8	237	7.56	0.07	12.9	153	3.26	0.54	48.2	1.91	0.0175
4.43	0.0001	82.8	0.00486	61.7	0.02	0.786	436	0.026				
10	SAG2-5	1.4	214	7.49	0.14	13.2	195	2.12	0.58	48.6	4.48	0.0137
4.13	0.00015	66.5	0.000582	55.6	0.02	0.216	593	0				
11	0943M	1.4	341	7.07	0.27	15.4	201	4.60	0.06	62.5	0.029	0.00079
8.34	0.00782	172	0.00678	151.0	3.71	0.05	603	0				
12	0951R	4.3	317	6.98	0.47	15.2	185	0.02	0.04	60.6	0.005	0.00181
8.32	0.00796	167	0.0255	141.0	3.78	0.05	556	0				
13	SAG1-1	0.5	209	7.57	0.20	14.2	131	4.8	8.0	45.7	0.738	0.02740
4.04	0.00012	98.1	0.00120	72.0	0.02	0.281	446	0				
14	SAG1-2	2.1	229	7.76	0.19	13.9	151	0.95	0.06	49.6	4.2	0.01940
4.81	0.0001	122	0.00662	86.4	0.02	0.786	474	0				
15	SAG1-3	1.9	180	7.65	0.22	13.9	184	1.11	0.06	53.1	6.13	0.02190
4.89	0.00013	125	0.00440	88.7	0.02	0.548	613	0				
16	SAG1-4	1.3	149	7.53	0.21	13.9	345	2.21	1.25	63.8	2.01	0.00620
3.71	0.0001	76.7	0.00138	34.9	0.02	0.109	1040	0				
17	SAG1-5	1.4	159	7.45	0.19	13.2	428	1.91	0.01	65.3	2.99	0.00806
2.99	0.00013	69.3	0.00143	29.2	0.02	0.152	1290	0				
18	SAG2-1	5.4	295	7.35	3.49	13.9	179	0.04	0.02	47.2	0.027	0.00200
4.17	0.00636	66.4	0.00715	53.5	2.39	0.05	394	0				
19	SAG2-2	5.2	292	7.38	2.38	13.6	177	0.07	0.06	47.2	0.03	0.00293
4.04	0.00567	66	0.00719	54.0	2.23	0.05	381	0				

20	SAG2-3	1.0	249	7.44	0.53	13.7	162	2.97	0.26	46.7	0.874	0.01000
4.36	0.00051	70.8	0.00623	56.9	0.02	0.379	397	0.064				
21	SAG2-4	0.7	250	7.75	0.28	13.6	145	4.60	0.09	48.4	2.11	0.01660
4.32	0.0001	88.8	0.00370	66.2	0.02	0.836	426	0				
22	SAG2-5	0.9	137	7.69	0.18	13.8	236	2.98	0.06	56.4	6.5	0.01730
4.61	0.00014	74.1	0.00303	46.0	0.02	0.243	769	0				

SELECTED_OUTPUT

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percent_error

saturation_indices Calcite Aragonite Dolomite(ordered) CaMoO4 CO2(g) Ferrihydrite Rhodochrosite Siderite FeSe Semetal(am) Uraninite

totals Se Se(4) Se(6) U U(4) U(6)

END

Beginning of initial solution calculations.

Initial solution 1. SAG1-1

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

Elements	Molality	Moles
Alkalinity	4.100e-03	4.100e-03
Ca	3.372e-03	3.372e-03
Cl	2.050e-03	2.050e-03
Fe(2)	5.915e-05	5.915e-05
Fe(3)	2.079e-04	2.079e-04
K	1.021e-04	1.021e-04
Mg	1.874e-03	1.874e-03
Mn	1.496e-05	1.496e-05
Mo	4.267e-07	4.267e-07
N(-3)	1.851e-05	1.851e-05
N(5)	1.429e-06	1.429e-06
Na	4.167e-03	4.167e-03
O(0)	9.384e-06	9.384e-06
S(6)	4.157e-03	4.157e-03
Se	2.916e-09	2.916e-09
U	7.359e-09	7.359e-09

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

pH = 7.430
pe = 0.400
Activity of water = 1.000
Ionic strength (mol/kgw) = 2.039e-02
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 4.410e-03
Total CO2 (mol/kg) = 4.410e-03
Temperature (°C) = 13.00
Electrical balance (eq) = 6.674e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 2.60
Iterations = 13
Total H = 1.110189e+02
Total O = 5.553714e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	3.9228	0.2227
N(-3)/N(5)	6.1785	0.3508
O(-2)/O(0)	13.6208	0.7733

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.214e-07	1.054e-07	-6.916	-6.977	-0.061	(0)	
H+	4.260e-08	3.715e-08	-7.371	-7.430	-0.059	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	
C(4)	4.410e-03						
HCO3-	3.933e-03	3.449e-03	-2.405	-2.462	-0.057	(0)	
H2CO3	3.365e-04	3.365e-04	-3.473	-3.473	0.000	(0)	
CaHCO3+	8.109e-05	7.131e-05	-4.091	-4.147	-0.056	(0)	
MgHCO3+	3.417e-05	2.975e-05	-4.466	-4.526	-0.060	(0)	
NaHCO3	8.785e-06	8.785e-06	-5.056	-5.056	0.000	(0)	
CaCO3	6.402e-06	6.402e-06	-5.194	-5.194	0.000	(0)	
CO3-2	5.878e-06	3.400e-06	-5.231	-5.469	-0.238	(0)	
MgCO3	2.082e-06	2.082e-06	-5.682	-5.682	0.000	(0)	
FeHCO3+	9.606e-07	8.448e-07	-6.017	-6.073	-0.056	(0)	
MnHCO3+	4.792e-07	4.194e-07	-6.319	-6.377	-0.058	(0)	
NaCO3-	3.657e-07	3.207e-07	-6.437	-6.494	-0.057	(0)	
Ca2UO2(CO3)3	5.451e-09	5.476e-09	-8.264	-8.262	0.002	(0)	
CaUO2(CO3)3-2	1.836e-09	1.062e-09	-8.736	-8.974	-0.238	(0)	
UO2(CO3)3-4	4.902e-11	3.528e-12	-10.310	-11.452	-1.143	(0)	
UO2(CO3)2-2	1.550e-11	8.030e-12	-10.810	-11.095	-0.286	(0)	
MgUO2(CO3)3-2	7.356e-12	4.255e-12	-11.133	-11.371	-0.238	(0)	
UO2CO3	1.450e-13	1.450e-13	-12.839	-12.839	0.000	(0)	
(UO2)2CO3(OH)3-	1.631e-18	1.423e-18	-17.787	-17.847	-0.059	(0)	
(UO2)3(CO3)6-6	1.159e-27	8.400e-30	-26.936	-29.076	-2.140	(0)	
Ca	3.372e-03						
Ca+2	2.692e-03	1.557e-03	-2.570	-2.808	-0.238	(0)	
CaSO4	5.918e-04	5.918e-04	-3.228	-3.228	0.000	(0)	
CaHCO3+	8.109e-05	7.131e-05	-4.091	-4.147	-0.056	(0)	
CaCO3	6.402e-06	6.402e-06	-5.194	-5.194	0.000	(0)	
CaNO3+	7.884e-09	6.689e-09	-8.103	-8.175	-0.071	(0)	
Ca2UO2(CO3)3	5.451e-09	5.476e-09	-8.264	-8.262	0.002	(0)	
CaOH+	3.236e-09	2.846e-09	-8.490	-8.546	-0.056	(0)	
CaUO2(CO3)3-2	1.836e-09	1.062e-09	-8.736	-8.974	-0.238	(0)	
CaNH3+2	9.050e-10	4.688e-10	-9.043	-9.329	-0.286	(0)	
Ca(NH3)2+2	8.614e-17	4.462e-17	-16.065	-16.350	-0.286	(0)	
Cl	2.050e-03						
Cl-	2.050e-03	1.788e-03	-2.688	-2.748	-0.059	(0)	
MnCl+	1.677e-08	1.467e-08	-7.776	-7.833	-0.058	(0)	
MnCl2	3.705e-11	3.705e-11	-10.431	-10.431	0.000	(0)	
MnCl3-	2.084e-14	1.824e-14	-13.681	-13.739	-0.058	(0)	
FeCl+2	5.865e-16	3.441e-16	-15.232	-15.463	-0.232	(0)	
FeCl2+	4.632e-18	4.054e-18	-17.334	-17.392	-0.058	(0)	
UO2Cl+	2.989e-20	2.536e-20	-19.524	-19.596	-0.071	(0)	
FeCl3	7.246e-22	7.246e-22	-21.140	-21.140	0.000	(0)	
UO2Cl2	2.732e-24	2.745e-24	-23.563	-23.561	0.002	(0)	
UCl+3	3.600e-38	8.194e-39	-37.444	-38.087	-0.643	(0)	
Fe(2)	5.915e-05						
Fe+2	4.808e-05	2.490e-05	-4.318	-4.604	-0.286	(0)	
FeSO4	9.987e-06	9.987e-06	-5.001	-5.001	0.000	(0)	
FeHCO3+	9.606e-07	8.448e-07	-6.017	-6.073	-0.056	(0)	
FeOH+	1.194e-07	1.045e-07	-6.923	-6.981	-0.058	(0)	
Fe(OH)2	7.642e-12	7.642e-12	-11.117	-11.117	0.000	(0)	
Fe(OH)3-	6.667e-13	5.835e-13	-12.176	-12.234	-0.058	(0)	
Fe(3)	2.079e-04						
Fe(OH)2+	1.977e-04	1.734e-04	-3.704	-3.761	-0.057	(0)	
Fe(OH)3	8.716e-06	8.716e-06	-5.060	-5.060	0.000	(0)	
Fe(OH)4-	1.451e-06	1.273e-06	-5.838	-5.895	-0.057	(0)	
FeOH+2	1.383e-09	8.110e-10	-8.859	-9.091	-0.232	(0)	
FeSO4+	1.477e-13	1.293e-13	-12.830	-12.888	-0.058	(0)	
Fe+3	3.223e-14	9.404e-15	-13.492	-14.027	-0.535	(0)	
Fe(SO4)2-	6.723e-15	5.703e-15	-14.172	-14.244	-0.071	(0)	
FeCl+2	5.865e-16	3.441e-16	-15.232	-15.463	-0.232	(0)	
Fe2(OH)2+4	4.697e-16	3.381e-17	-15.328	-16.471	-1.143	(0)	
FeCl2+	4.632e-18	4.054e-18	-17.334	-17.392	-0.058	(0)	

Fe3(OH)4+5	4.547e-18	7.450e-20	-17.342	-19.128	-1.786	(0)
FeNO3+2	4.209e-19	2.180e-19	-18.376	-18.662	-0.286	(0)
FeHSeO3+2	6.652e-20	3.445e-20	-19.177	-19.463	-0.286	(0)
FeCl3	7.246e-22	7.246e-22	-21.140	-21.140	0.000	(0)
H(0)	3.492e-19					
H2	1.746e-19	1.754e-19	-18.758	-18.756	0.002	(0)
K	1.021e-04					
K+	1.009e-04	8.800e-05	-3.996	-4.056	-0.059	(0)
KSO4-	1.240e-06	1.087e-06	-5.907	-5.964	-0.057	(0)
Mg	1.874e-03					
Mg+2	1.559e-03	9.019e-04	-2.807	-3.045	-0.238	(0)
MgSO4	2.783e-04	2.783e-04	-3.556	-3.556	0.000	(0)
MgHCO3+	3.417e-05	2.975e-05	-4.466	-4.526	-0.060	(0)
MgCO3	2.082e-06	2.082e-06	-5.682	-5.682	0.000	(0)
MgOH+	3.505e-08	3.089e-08	-7.455	-7.510	-0.055	(0)
MgUO2(CO3)3-2	7.356e-12	4.255e-12	-11.133	-11.371	-0.238	(0)
Mn(2)	1.496e-05					
Mn+2	1.259e-05	6.521e-06	-4.900	-5.186	-0.286	(0)
MnSO4	1.872e-06	1.872e-06	-5.728	-5.728	0.000	(0)
MnHCO3+	4.792e-07	4.194e-07	-6.319	-6.377	-0.058	(0)
MnCl+	1.677e-08	1.467e-08	-7.776	-7.833	-0.058	(0)
MnOH+	1.973e-09	1.726e-09	-8.705	-8.763	-0.058	(0)
MnCl2	3.705e-11	3.705e-11	-10.431	-10.431	0.000	(0)
MnNO3+	1.510e-11	1.281e-11	-10.821	-10.892	-0.071	(0)
MnCl3-	2.084e-14	1.824e-14	-13.681	-13.739	-0.058	(0)
MnSe	1.162e-14	1.162e-14	-13.935	-13.935	0.000	(0)
Mn(NO3)2	4.102e-17	4.102e-17	-16.387	-16.387	0.000	(0)
Mn(OH)3-	2.300e-18	2.013e-18	-17.638	-17.696	-0.058	(0)
Mn(OH)4-2	3.002e-24	1.761e-24	-23.523	-23.754	-0.232	(0)
MnSeO4	5.898e-27	5.898e-27	-26.229	-26.229	0.000	(0)
Mn(3)	4.048e-31					
Mn+3	4.048e-31	1.181e-31	-30.393	-30.928	-0.535	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-67.561	-67.792	-0.232	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-77.522	-77.584	-0.063	(0)
Mo	4.267e-07					
MoO4-2	4.266e-07	2.467e-07	-6.370	-6.608	-0.238	(0)
HMoO4-	1.533e-10	1.300e-10	-9.814	-9.886	-0.071	(0)
H2MoO4	7.706e-14	7.706e-14	-13.113	-13.113	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-48.457	-51.029	-2.571	(0)
HMo7O24-5	0.000e+00	0.000e+00	-50.360	-52.145	-1.786	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-53.672	-54.815	-1.143	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-58.342	-58.985	-0.643	(0)
N(-3)	1.851e-05					
NH4+	1.805e-05	1.558e-05	-4.743	-4.807	-0.064	(0)
NH4SO4-	3.568e-07	3.122e-07	-6.448	-6.506	-0.058	(0)
NH3	9.921e-08	9.921e-08	-7.003	-7.003	0.000	(0)
CaNH3+2	9.050e-10	4.688e-10	-9.043	-9.329	-0.286	(0)
Ca(NH3)2+2	8.614e-17	4.462e-17	-16.065	-16.350	-0.286	(0)
N(5)	1.429e-06					
NO3-	1.421e-06	1.240e-06	-5.847	-5.907	-0.059	(0)
CaNO3+	7.884e-09	6.689e-09	-8.103	-8.175	-0.071	(0)
MnNO3+	1.510e-11	1.281e-11	-10.821	-10.892	-0.071	(0)
Mn(NO3)2	4.102e-17	4.102e-17	-16.387	-16.387	0.000	(0)
FeNO3+2	4.209e-19	2.180e-19	-18.376	-18.662	-0.286	(0)
UO2NO3+	4.095e-23	3.474e-23	-22.388	-22.459	-0.071	(0)
Na	4.167e-03					
Na+	4.117e-03	3.591e-03	-2.385	-2.445	-0.059	(0)
NaSO4-	4.044e-05	3.546e-05	-4.393	-4.450	-0.057	(0)
NaHCO3	8.785e-06	8.785e-06	-5.056	-5.056	0.000	(0)
NaCO3-	3.657e-07	3.207e-07	-6.437	-6.494	-0.057	(0)
O(0)	9.384e-06					
O2	4.692e-06	4.714e-06	-5.329	-5.327	0.002	(0)
S(6)	4.157e-03					
SO4-2	3.234e-03	1.870e-03	-2.490	-2.728	-0.238	(0)

CaSO4	5.918e-04	5.918e-04	-3.228	-3.228	0.000	(0)
MgSO4	2.783e-04	2.783e-04	-3.556	-3.556	0.000	(0)
NaSO4-	4.044e-05	3.546e-05	-4.393	-4.450	-0.057	(0)
FeSO4	9.987e-06	9.987e-06	-5.001	-5.001	0.000	(0)
MnSO4	1.872e-06	1.872e-06	-5.728	-5.728	0.000	(0)
KSO4-	1.240e-06	1.087e-06	-5.907	-5.964	-0.057	(0)
NH4SO4-	3.568e-07	3.122e-07	-6.448	-6.506	-0.058	(0)
HSO4-	5.362e-09	4.680e-09	-8.271	-8.330	-0.059	(0)
FeSO4+	1.477e-13	1.293e-13	-12.830	-12.888	-0.058	(0)
Fe(SO4)2-	6.723e-15	5.703e-15	-14.172	-14.244	-0.071	(0)
UO2SO4	2.314e-17	2.314e-17	-16.636	-16.636	0.000	(0)
UO2(SO4)2-2	8.123e-19	4.207e-19	-18.090	-18.376	-0.286	(0)
U(SO4)2	4.128e-33	4.128e-33	-32.384	-32.384	0.000	(0)
USO4+2	8.187e-34	4.241e-34	-33.087	-33.373	-0.286	(0)
Se(-2)	1.896e-11					
HSe-	1.894e-11	1.607e-11	-10.723	-10.794	-0.071	(0)
MnSe	1.162e-14	1.162e-14	-13.935	-13.935	0.000	(0)
H2Se	4.383e-15	4.383e-15	-14.358	-14.358	0.000	(0)
Se-2	3.700e-19	1.916e-19	-18.432	-18.717	-0.286	(0)
Se(4)	2.897e-09					
HSeO3-	2.495e-09	2.116e-09	-8.603	-8.674	-0.071	(0)
SeO3-2	4.021e-10	2.083e-10	-9.396	-9.681	-0.286	(0)
H2SeO3	3.020e-14	3.020e-14	-13.520	-13.520	0.000	(0)
FeHSeO3+2	6.652e-20	3.445e-20	-19.177	-19.463	-0.286	(0)
Se(6)	7.369e-24					
SeO4-2	7.363e-24	4.259e-24	-23.133	-23.371	-0.238	(0)
MnSeO4	5.898e-27	5.898e-27	-26.229	-26.229	0.000	(0)
HSeO4-	6.335e-30	5.374e-30	-29.198	-29.270	-0.071	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-46.489	-47.132	-0.643	(0)
U(4)	1.170e-14					
U(OH)5-	1.168e-14	9.908e-15	-13.933	-14.004	-0.071	(0)
U(OH)4	1.882e-17	1.882e-17	-16.725	-16.725	0.000	(0)
U(OH)3+	3.501e-21	2.970e-21	-20.456	-20.527	-0.071	(0)
U(OH)2+2	1.395e-25	7.228e-26	-24.855	-25.141	-0.286	(0)
UOH+3	8.684e-31	1.977e-31	-30.061	-30.704	-0.643	(0)
U(SO4)2	4.128e-33	4.128e-33	-32.384	-32.384	0.000	(0)
USO4+2	8.187e-34	4.241e-34	-33.087	-33.373	-0.286	(0)
U+4	9.059e-37	6.521e-38	-36.043	-37.186	-1.143	(0)
UCl+3	3.600e-38	8.194e-39	-37.444	-38.087	-0.643	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-123.036	-128.821	-5.785	(0)
U(5)	4.142e-15					
UO2+	4.142e-15	3.514e-15	-14.383	-14.454	-0.071	(0)
U(6)	7.359e-09					
Ca2UO2(CO3)3	5.451e-09	5.476e-09	-8.264	-8.262	0.002	(0)
CaUO2(CO3)3-2	1.836e-09	1.062e-09	-8.736	-8.974	-0.238	(0)
UO2(CO3)3-4	4.902e-11	3.528e-12	-10.310	-11.452	-1.143	(0)
UO2(CO3)2-2	1.550e-11	8.030e-12	-10.810	-11.095	-0.286	(0)
MgUO2(CO3)3-2	7.356e-12	4.255e-12	-11.133	-11.371	-0.238	(0)
UO2(OH)2	4.003e-13	4.022e-13	-12.398	-12.396	0.002	(0)
UO2CO3	1.450e-13	1.450e-13	-12.839	-12.839	0.000	(0)
UO2(OH)3-	1.537e-14	1.340e-14	-13.813	-13.873	-0.059	(0)
UO2OH+	2.053e-16	1.742e-16	-15.688	-15.759	-0.071	(0)
UO2SO4	2.314e-17	2.314e-17	-16.636	-16.636	0.000	(0)
UO2+2	1.982e-17	1.146e-17	-16.703	-16.941	-0.238	(0)
(UO2)2CO3(OH)3-	1.631e-18	1.423e-18	-17.787	-17.847	-0.059	(0)
UO2(SO4)2-2	8.123e-19	4.207e-19	-18.090	-18.376	-0.286	(0)
UO2Cl+	2.989e-20	2.536e-20	-19.524	-19.596	-0.071	(0)
UO2(OH)4-2	9.715e-21	5.619e-21	-20.013	-20.250	-0.238	(0)
UO2NO3+	4.095e-23	3.474e-23	-22.388	-22.459	-0.071	(0)
UO2Cl2	2.732e-24	2.745e-24	-23.563	-23.561	0.002	(0)
(UO2)2(OH)2+2	2.415e-25	1.251e-25	-24.617	-24.903	-0.286	(0)
(UO2)3(CO3)6-6	1.159e-27	8.400e-30	-26.936	-29.076	-2.140	(0)
(UO2)2OH+3	2.379e-29	6.940e-30	-28.624	-29.159	-0.535	(0)
(UO2)3(OH)7-	1.569e-30	1.369e-30	-29.804	-29.864	-0.059	(0)
(UO2)3(OH)5+	1.047e-30	8.883e-31	-29.980	-30.051	-0.071	(0)

(UO2)3(OH)4+2 1.608e-33 9.301e-34 -32.794 -33.031 -0.238 (0)
 (UO2)4(OH)7+ 2.265e-38 1.975e-38 -37.645 -37.704 -0.059 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-33.44	-32.99	0.45 (NH4)2SeO4
Anhydrite	-1.23	-5.54	-4.31 CaSO4
Aragonite	-0.06	-8.28	-8.21 CaCO3
Artinite	-7.18	3.30	10.48 MgCO3:Mg(OH)2:3H2O
Birnessite	-18.90	-0.81	18.09 MnO2
Bixbyite	-17.55	-17.28	0.27 Mn2O3
Brucite	-5.87	11.81	17.68 Mg(OH)2
Calcite	0.15	-8.28	-8.42 CaCO3
CaMoO4	-1.48	-9.42	-7.94 CaMoO4
CaSeO3:2H2O	-7.01	-4.05	2.96 CaSeO3:2H2O
CaSeO4:2H2O	-23.22	-26.18	-2.96 CaSeO4:2H2O
CH4(g)	-40.03	-82.97	-42.93 CH4
CO2(g)	-2.15	-20.33	-18.18 CO2
Dolomite(disordered)	-0.59	-16.79	-16.20 CaMg(CO3)2
Dolomite(ordered)	0.01	-16.79	-16.80 CaMg(CO3)2
Epsomite	-3.56	-5.77	-2.21 MgSO4:7H2O
Fe(OH)2	-3.31	10.26	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	8.25	5.21	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-1.13	0.42	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-11.16	-31.79	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-34.28	-36.24	-1.96 Fe2(SO4)3
Fe3(OH)8	6.56	26.78	20.22 Fe3(OH)8
FeMoO4	-1.20	-11.21	-10.01 FeMoO4
Ferrihydrite	4.53	8.26	3.73 Fe(OH)3
Ferroselite	8.41	-10.53	-18.94 FeSe2
FeSe	3.05	-7.97	-11.02 FeSe
Goethite	7.33	8.26	0.94 FeOOH
Gummite	-10.35	-2.08	8.27 UO3
Gypsum	-0.92	-5.54	-4.62 CaSO4:2H2O
H-Jarosite	0.02	-10.39	-10.40 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-8.23	-21.47	-13.24 H2MoO4
H2Se(g)	-13.38	-18.22	-4.85 H2Se
Halite	-6.77	-5.19	1.58 NaCl
Hausmannite	-19.44	44.68	64.12 Mn3O4
Hematite	17.00	16.53	-0.47 Fe2O3
Huntite	-4.64	-33.82	-29.18 CaMg3(CO3)4
Hydromagnesite	-15.08	-22.24	-7.16 Mg5(CO3)4(OH)2:4H2O
K-Jarosite	6.83	-7.01	-13.84 KFe3(SO4)2(OH)6
K2MoO4	-18.01	-14.72	3.29 K2MoO4
K2SeO4	-30.75	-31.48	-0.73 K2SeO4
Lepidocrocite	6.89	8.26	1.37 FeOOH
Lime	-22.07	12.05	34.12 CaO
Maghemite	10.14	16.53	6.39 Fe2O3
Magnesioferrite	9.43	28.34	18.91 Fe2MgO4
Magnesite	-0.91	-8.51	-7.61 MgCO3
Magnetite	21.85	26.78	4.93 Fe3O4
Manganite	-7.84	17.50	25.34 MnOOH
Melanterite	-4.97	-7.33	-2.36 FeSO4:7H2O
Mg(OH)2(active)	-6.98	11.81	18.79 Mg(OH)2
MgMoO4	-7.80	-9.65	-1.85 MgMoO4
MgSeO3:6H2O	-7.31	-4.29	3.02 MgSeO3:6H2O
MgSeO4:6H2O	-25.22	-26.42	-1.20 MgSeO4:6H2O
Mirabilite	-5.92	-7.62	-1.70 Na2SO4:10H2O
Mn2(SO4)3	-65.53	-70.04	-4.51 Mn2(SO4)3
MnCl2:4H2O	-13.48	-10.68	2.79 MnCl2:4H2O
MnSe	-12.77	-8.55	4.22 MnSe
MnSeO3	-7.56	-6.43	1.13 MnSeO3
MnSeO3:2H2O	-7.35	-6.43	0.92 MnSeO3:2H2O
MnSeO4:5H2O	-26.51	-28.56	-2.05 MnSeO4:5H2O

MnSO4 -10.97 -7.91 3.06 MnSO4
MoO3 -13.47 -21.47 -8.00 MoO3
Na-Jarosite 4.69 -5.40 -10.09 NaFe3(SO4)2(OH)6
Na2Mo2O7 -15.96 -32.97 -17.01 Na2Mo2O7
Na2MoO4 -13.06 -11.50 1.56 Na2MoO4
Na2MoO4:2H2O -12.72 -11.50 1.22 Na2MoO4:2H2O
Na2SeO3:5H2O -16.43 -6.13 10.30 Na2SeO3:5H2O
Na2SeO4 -29.54 -28.26 1.28 Na2SeO4
Natron -8.56 -10.36 -1.79 Na2CO3:10H2O
Nesquehonite -4.02 -8.51 -4.49 MgCO3:3H2O
Nsutite -18.31 -0.81 17.50 MnO2
O2(g) -55.97 31.32 87.29 O2
Periclase -10.88 11.82 22.70 MgO
Portlandite -11.70 12.05 23.75 Ca(OH)2
Pyrochroite -6.23 9.67 15.91 Mn(OH)2
Pyrolusite -18.04 25.33 43.38 MnO2
Rhodochrosite -0.09 -10.65 -10.57 MnCO3
Rutherfordine -7.93 -22.41 -14.48 UO2CO3
Schoepite -8.44 -2.08 6.36 UO2(OH)2:H2O
Semetal(am) 4.63 -2.56 -7.19 Se
Semetal(hex) 5.26 -2.56 -7.83 Se
SeO2 -16.22 -16.10 0.11 SeO2
SeO3 -60.35 -38.23 22.12 SeO3
Siderite 0.05 -10.07 -10.12 FeCO3
Thenardite -8.01 -7.62 0.39 Na2SO4
Thermonatrite -11.07 -10.36 0.71 Na2CO3:H2O
U3O8 -15.73 8.92 24.65 U3O8
U4O9 -14.32 -14.20 0.12 U4O9
UO2(am) -9.21 -7.47 1.74 UO2
UO2(NO3)2 -41.51 -28.75 12.76 UO2(NO3)2
UO2(NO3)2:2H2O -33.79 -28.75 5.04 UO2(NO3)2:2H2O
UO2(NO3)2:3H2O -32.21 -28.75 3.46 UO2(NO3)2:3H2O
UO2(NO3)2:6H2O -30.65 -28.75 1.89 UO2(NO3)2:6H2O
UO2(OH)2(beta) -8.11 -2.08 6.03 UO2(OH)2
UO2SeO4:4H2O -38.06 -40.31 -2.25 UO2SeO4:4H2O
UO3 -10.38 -2.08 8.30 UO3
Uraninite -3.37 -7.47 -4.10 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 2. SAG1-2

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

Elements	Molality	Moles
Alkalinity	4.021e-03	4.021e-03
Ca	3.597e-03	3.597e-03
Cl	2.663e-03	2.663e-03
Fe(2)	1.595e-05	1.595e-05
Fe(3)	5.378e-07	5.378e-07
K	1.234e-04	1.234e-04
Mg	1.952e-03	1.952e-03
Mn	7.890e-05	7.890e-05
Mo	3.047e-07	3.047e-07
N(-3)	5.282e-05	5.282e-05
N(5)	1.429e-06	1.429e-06
Na	5.356e-03	5.356e-03
O(0)	7.508e-06	7.508e-06
S(6)	4.804e-03	4.804e-03
Se	2.662e-09	2.662e-09
U	2.957e-08	2.957e-08

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

pH = 7.590
 pe = 1.900
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.254e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 4.222e-03
 Total CO2 (mol/kg) = 4.222e-03
 Temperature (°C) = 13.70
 Electrical balance (eq) = 5.274e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.84
 Iterations = 14 (27 overall)
 Total H = 1.110183e+02
 Total O = 5.553873e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	1.5714	0.0894
N(-3)/N(5)	5.8783	0.3346
O(-2)/O(0)	13.3831	0.7617

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.870e-07	1.613e-07	-6.728	-6.792	-0.064	(0)	
H+	2.965e-08	2.570e-08	-7.528	-7.590	-0.062	0.00	
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.03	
C(4)	4.222e-03						
HCO3-	3.847e-03	3.355e-03	-2.415	-2.474	-0.059	(0)	
H2CO3	2.243e-04	2.243e-04	-3.649	-3.649	0.000	(0)	
CaHCO3+	8.275e-05	7.240e-05	-4.082	-4.140	-0.058	(0)	
MgHCO3+	3.365e-05	2.912e-05	-4.473	-4.536	-0.063	(0)	
NaHCO3	1.075e-05	1.075e-05	-4.968	-4.968	0.000	(0)	
CaCO3	9.496e-06	9.496e-06	-5.022	-5.022	0.000	(0)	
CO3-2	8.586e-06	4.852e-06	-5.066	-5.314	-0.248	(0)	
MgCO3	3.015e-06	3.015e-06	-5.521	-5.521	0.000	(0)	
MnHCO3+	2.372e-06	2.065e-06	-5.625	-5.685	-0.060	(0)	
NaCO3-	6.560e-07	5.721e-07	-6.183	-6.243	-0.059	(0)	
FeHCO3+	2.443e-07	2.138e-07	-6.612	-6.670	-0.058	(0)	
Ca2UO2(CO3)3	2.190e-08	2.201e-08	-7.660	-7.657	0.002	(0)	
CaUO2(CO3)3-2	7.387e-09	4.174e-09	-8.132	-8.379	-0.248	(0)	
UO2(CO3)3-4	2.076e-10	1.302e-11	-9.683	-10.885	-1.203	(0)	
UO2(CO3)2-2	4.394e-11	2.199e-11	-10.357	-10.658	-0.301	(0)	
MgUO2(CO3)3-2	2.901e-11	1.639e-11	-10.537	-10.785	-0.248	(0)	
UO2CO3	2.748e-13	2.748e-13	-12.561	-12.561	0.000	(0)	
(UO2)2CO3(OH)3-	1.219e-17	1.057e-17	-16.914	-16.976	-0.062	(0)	
(UO2)3(CO3)6-6	2.554e-26	1.500e-28	-25.593	-27.824	-2.231	(0)	
Ca	3.597e-03						
Ca+2	2.818e-03	1.593e-03	-2.550	-2.798	-0.248	(0)	
CaSO4	6.863e-04	6.863e-04	-3.163	-3.163	0.000	(0)	
CaHCO3+	8.275e-05	7.240e-05	-4.082	-4.140	-0.058	(0)	
CaCO3	9.496e-06	9.496e-06	-5.022	-5.022	0.000	(0)	
Ca2UO2(CO3)3	2.190e-08	2.201e-08	-7.660	-7.657	0.002	(0)	
CaNO3+	8.040e-09	6.762e-09	-8.095	-8.170	-0.075	(0)	
CaUO2(CO3)3-2	7.387e-09	4.174e-09	-8.132	-8.379	-0.248	(0)	
CaOH+	5.135e-09	4.493e-09	-8.289	-8.348	-0.058	(0)	
CaNH3+2	3.904e-09	1.953e-09	-8.409	-8.709	-0.301	(0)	
Ca(NH3)2+2	1.514e-15	7.578e-16	-14.820	-15.120	-0.301	(0)	
Cl	2.663e-03						
Cl-	2.663e-03	2.309e-03	-2.575	-2.637	-0.062	(0)	
MnCl+	1.098e-07	9.553e-08	-6.960	-7.020	-0.060	(0)	
MnCl2	3.115e-10	3.115e-10	-9.507	-9.507	0.000	(0)	
MnCl3-	2.276e-13	1.981e-13	-12.643	-12.703	-0.060	(0)	

FeCl+2	9.458e-19	5.424e-19	-18.024	-18.266	-0.241	(0)
UO2Cl+	5.235e-20	4.403e-20	-19.281	-19.356	-0.075	(0)
FeCl2+	9.263e-21	8.061e-21	-20.033	-20.094	-0.060	(0)
UO2Cl2	6.025e-24	6.056e-24	-23.220	-23.218	0.002	(0)
FeCl3	1.861e-24	1.861e-24	-23.730	-23.730	0.000	(0)
UCl+3	0.000e+00	0.000e+00	-40.891	-41.567	-0.677	(0)
Fe(2)	1.595e-05					
Fe+2	1.276e-05	6.383e-06	-4.894	-5.195	-0.301	(0)
FeSO4	2.906e-06	2.906e-06	-5.537	-5.537	0.000	(0)
FeHCO3+	2.443e-07	2.138e-07	-6.612	-6.670	-0.058	(0)
FeOH+	4.711e-08	4.099e-08	-7.327	-7.387	-0.060	(0)
Fe(OH)2	4.626e-12	4.626e-12	-11.335	-11.335	0.000	(0)
Fe(OH)3-	5.908e-13	5.141e-13	-12.229	-12.289	-0.060	(0)
Fe(3)	5.378e-07					
Fe(OH)2+	4.953e-07	4.319e-07	-6.305	-6.365	-0.059	(0)
Fe(OH)3	3.491e-08	3.491e-08	-7.457	-7.457	0.000	(0)
Fe(OH)4-	7.595e-09	6.623e-09	-8.119	-8.179	-0.059	(0)
FeOH+2	2.544e-12	1.459e-12	-11.595	-11.836	-0.241	(0)
FeSO4+	2.046e-16	1.781e-16	-15.689	-15.749	-0.060	(0)
Fe+3	4.050e-17	1.121e-17	-16.393	-16.950	-0.558	(0)
Fe(SO4)2-	1.045e-17	8.793e-18	-16.981	-17.056	-0.075	(0)
FeCl+2	9.458e-19	5.424e-19	-18.024	-18.266	-0.241	(0)
FeCl2+	9.263e-21	8.061e-21	-20.033	-20.094	-0.060	(0)
Fe2(OH)2+4	1.699e-21	1.065e-22	-20.770	-21.973	-1.203	(0)
FeNO3+2	4.971e-22	2.488e-22	-21.304	-21.604	-0.301	(0)
FeHSeO3+2	7.185e-23	3.595e-23	-22.144	-22.444	-0.301	(0)
FeCl3	1.861e-24	1.861e-24	-23.730	-23.730	0.000	(0)
Fe3(OH)4+5	4.462e-26	5.893e-28	-25.350	-27.230	-1.879	(0)
H(0)	1.658e-22					
H2	8.290e-23	8.333e-23	-22.081	-22.079	0.002	(0)
K	1.234e-04					
K+	1.217e-04	1.055e-04	-3.915	-3.977	-0.062	(0)
KSO4-	1.690e-06	1.474e-06	-5.772	-5.831	-0.059	(0)
Mg	1.952e-03					
Mg+2	1.600e-03	9.040e-04	-2.796	-3.044	-0.248	(0)
MgSO4	3.159e-04	3.159e-04	-3.500	-3.500	0.000	(0)
MgHCO3+	3.365e-05	2.912e-05	-4.473	-4.536	-0.063	(0)
MgCO3	3.015e-06	3.015e-06	-5.521	-5.521	0.000	(0)
MgOH+	5.470e-08	4.798e-08	-7.262	-7.319	-0.057	(0)
MgUO2(CO3)3-2	2.901e-11	1.639e-11	-10.537	-10.785	-0.248	(0)
Mn(2)	7.890e-05					
Mn+2	6.568e-05	3.287e-05	-4.183	-4.483	-0.301	(0)
MnSO4	1.072e-05	1.072e-05	-4.970	-4.970	0.000	(0)
MnHCO3+	2.372e-06	2.065e-06	-5.625	-5.685	-0.060	(0)
MnCl+	1.098e-07	9.553e-08	-6.960	-7.020	-0.060	(0)
MnOH+	1.530e-08	1.332e-08	-7.815	-7.876	-0.060	(0)
MnCl2	3.115e-10	3.115e-10	-9.507	-9.507	0.000	(0)
MnNO3+	7.633e-11	6.420e-11	-10.117	-10.192	-0.075	(0)
MnCl3-	2.276e-13	1.981e-13	-12.643	-12.703	-0.060	(0)
Mn(NO3)2	2.040e-16	2.040e-16	-15.690	-15.690	0.000	(0)
Mn(OH)3-	3.521e-17	3.064e-17	-16.453	-16.514	-0.060	(0)
MnSeO4	9.551e-23	9.551e-23	-22.020	-22.020	0.000	(0)
Mn(OH)4-2	6.755e-23	3.874e-23	-22.170	-22.412	-0.241	(0)
MnSe	7.922e-24	7.922e-24	-23.101	-23.101	0.000	(0)
Mn(3)	7.596e-29					
Mn+3	7.596e-29	2.103e-29	-28.119	-28.677	-0.558	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-59.252	-59.493	-0.241	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-67.670	-67.735	-0.066	(0)
Mo	3.047e-07					
MoO4-2	3.046e-07	1.721e-07	-6.516	-6.764	-0.248	(0)
HMoO4-	7.617e-11	6.407e-11	-10.118	-10.193	-0.075	(0)
H2MoO4	2.505e-14	2.505e-14	-13.601	-13.601	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-50.799	-53.505	-2.706	(0)
HMo7O24-5	0.000e+00	0.000e+00	-52.898	-54.777	-1.879	(0)

H2Mo7O24-4 0.000e+00 0.000e+00 -56.403 -57.606 -1.203 (0)
H3Mo7O24-3 0.000e+00 0.000e+00 -61.259 -61.936 -0.677 (0)
N(-3) 5.282e-05
NH4+ 5.125e-05 4.393e-05 -4.290 -4.357 -0.067 (0)
NH4SO4- 1.139e-06 9.912e-07 -5.943 -6.004 -0.060 (0)
NH3 4.264e-07 4.264e-07 -6.370 -6.370 0.000 (0)
CaNH3+2 3.904e-09 1.953e-09 -8.409 -8.709 -0.301 (0)
Ca(NH3)2+2 1.514e-15 7.578e-16 -14.820 -15.120 -0.301 (0)
N(5) 1.429e-06
NO3- 1.421e-06 1.232e-06 -5.847 -5.909 -0.062 (0)
CaNO3+ 8.040e-09 6.762e-09 -8.095 -8.170 -0.075 (0)
MnNO3+ 7.633e-11 6.420e-11 -10.117 -10.192 -0.075 (0)
Mn(NO3)2 2.040e-16 2.040e-16 -15.690 -15.690 0.000 (0)
FeNO3+2 4.971e-22 2.488e-22 -21.304 -21.604 -0.301 (0)
UO2NO3+ 5.364e-23 4.512e-23 -22.270 -22.346 -0.075 (0)
Na 5.356e-03
Na+ 5.286e-03 4.583e-03 -2.277 -2.339 -0.062 (0)
NaSO4- 5.850e-05 5.102e-05 -4.233 -4.292 -0.059 (0)
NaHCO3 1.075e-05 1.075e-05 -4.968 -4.968 0.000 (0)
NaCO3- 6.560e-07 5.721e-07 -6.183 -6.243 -0.059 (0)
O(0) 7.508e-06
O2 3.754e-06 3.774e-06 -5.425 -5.423 0.002 (0)
S(6) 4.804e-03
SO4-2 3.727e-03 2.106e-03 -2.429 -2.677 -0.248 (0)
CaSO4 6.863e-04 6.863e-04 -3.163 -3.163 0.000 (0)
MgSO4 3.159e-04 3.159e-04 -3.500 -3.500 0.000 (0)
NaSO4- 5.850e-05 5.102e-05 -4.233 -4.292 -0.059 (0)
MnSO4 1.072e-05 1.072e-05 -4.970 -4.970 0.000 (0)
FeSO4 2.906e-06 2.906e-06 -5.537 -5.537 0.000 (0)
KSO4- 1.690e-06 1.474e-06 -5.772 -5.831 -0.059 (0)
NH4SO4- 1.139e-06 9.912e-07 -5.943 -6.004 -0.060 (0)
HSO4- 4.297e-09 3.729e-09 -8.367 -8.428 -0.062 (0)
FeSO4+ 2.046e-16 1.781e-16 -15.689 -15.749 -0.060 (0)
UO2SO4 3.517e-17 3.517e-17 -16.454 -16.454 0.000 (0)
Fe(SO4)2- 1.045e-17 8.793e-18 -16.981 -17.056 -0.075 (0)
UO2(SO4)2-2 1.466e-18 7.336e-19 -17.834 -18.135 -0.301 (0)
U(SO4)2 1.415e-36 1.415e-36 -35.849 -35.849 0.000 (0)
USO4+2 2.515e-37 1.258e-37 -36.599 -36.900 -0.301 (0)
Se(-2) 1.796e-21
HSe- 1.787e-21 1.503e-21 -20.748 -20.823 -0.075 (0)
MnSe 7.922e-24 7.922e-24 -23.101 -23.101 0.000 (0)
H2Se 2.846e-25 2.846e-25 -24.546 -24.546 0.000 (0)
Se-2 5.441e-29 2.723e-29 -28.264 -28.565 -0.301 (0)
Se(4) 2.662e-09
HSeO3- 2.147e-09 1.805e-09 -8.668 -8.743 -0.075 (0)
SeO3-2 5.159e-10 2.582e-10 -9.287 -9.588 -0.301 (0)
H2SeO3 1.794e-14 1.794e-14 -13.746 -13.746 0.000 (0)
FeHSeO3+2 7.185e-23 3.595e-23 -22.144 -22.444 -0.301 (0)
Se(6) 2.396e-20
SeO4-2 2.386e-20 1.349e-20 -19.622 -19.870 -0.248 (0)
MnSeO4 9.551e-23 9.551e-23 -22.020 -22.020 0.000 (0)
HSeO4- 1.433e-26 1.205e-26 -25.844 -25.919 -0.075 (0)
U(3) 0.000e+00
U+3 0.000e+00 0.000e+00 -51.492 -52.169 -0.677 (0)
U(4) 2.189e-17
U(OH)5- 2.186e-17 1.839e-17 -16.660 -16.735 -0.075 (0)
U(OH)4 2.388e-20 2.388e-20 -19.622 -19.622 0.000 (0)
U(OH)3+ 3.072e-24 2.584e-24 -23.513 -23.588 -0.075 (0)
U(OH)2+2 8.511e-29 4.259e-29 -28.070 -28.371 -0.301 (0)
UOH+3 3.724e-34 7.843e-35 -33.429 -34.106 -0.677 (0)
U(SO4)2 1.415e-36 1.415e-36 -35.849 -35.849 0.000 (0)
USO4+2 2.515e-37 1.258e-37 -36.599 -36.900 -0.301 (0)
U+4 2.718e-40 0.000e+00 -39.566 -40.768 -1.203 (0)
UCl+3 0.000e+00 0.000e+00 -40.891 -41.567 -0.677 (0)
U6(OH)15+9 0.000e+00 0.000e+00 -141.829 -147.918 -6.089 (0)
U(5) 1.723e-16

UO2+ 1.723e-16 1.449e-16 -15.764 -15.839 -0.075 (0)
 U(6) 2.957e-08
 Ca2UO2(CO3)3 2.190e-08 2.201e-08 -7.660 -7.657 0.002 (0)
 CaUO2(CO3)3-2 7.387e-09 4.174e-09 -8.132 -8.379 -0.248 (0)
 UO2(CO3)3-4 2.076e-10 1.302e-11 -9.683 -10.885 -1.203 (0)
 UO2(CO3)2-2 4.394e-11 2.199e-11 -10.357 -10.658 -0.301 (0)
 MgUO2(CO3)3-2 2.901e-11 1.639e-11 -10.537 -10.785 -0.248 (0)
 UO2(OH)2 1.106e-12 1.111e-12 -11.956 -11.954 0.002 (0)
 UO2CO3 2.748e-13 2.748e-13 -12.561 -12.561 0.000 (0)
 UO2(OH)3- 6.173e-14 5.352e-14 -13.209 -13.271 -0.062 (0)
 UO2OH+ 4.158e-16 3.497e-16 -15.381 -15.456 -0.075 (0)
 UO2SO4 3.517e-17 3.517e-17 -16.454 -16.454 0.000 (0)
 UO2+2 2.683e-17 1.516e-17 -16.571 -16.819 -0.248 (0)
 (UO2)2CO3(OH)3- 1.219e-17 1.057e-17 -16.914 -16.976 -0.062 (0)
 UO2(SO4)2-2 1.466e-18 7.336e-19 -17.834 -18.135 -0.301 (0)
 UO2(OH)4-2 5.741e-20 3.244e-20 -19.241 -19.489 -0.248 (0)
 UO2Cl+ 5.235e-20 4.403e-20 -19.281 -19.356 -0.075 (0)
 UO2NO3+ 5.364e-23 4.512e-23 -22.270 -22.346 -0.075 (0)
 UO2Cl2 6.025e-24 6.056e-24 -23.220 -23.218 0.002 (0)
 (UO2)2(OH)2+2 9.536e-25 4.772e-25 -24.021 -24.321 -0.301 (0)
 (UO2)3(CO3)6-6 2.554e-26 1.500e-28 -25.593 -27.824 -2.231 (0)
 (UO2)2OH+3 6.339e-29 1.755e-29 -28.198 -28.756 -0.558 (0)
 (UO2)3(OH)7- 4.814e-29 4.174e-29 -28.318 -28.379 -0.062 (0)
 (UO2)3(OH)5+ 1.722e-29 1.449e-29 -28.764 -28.839 -0.075 (0)
 (UO2)3(OH)4+2 1.662e-32 9.393e-33 -31.779 -32.027 -0.248 (0)
 (UO2)4(OH)7+ 9.190e-37 7.968e-37 -36.037 -36.099 -0.062 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-29.03	-28.58	0.45 (NH4)2SeO4
Anhydrite	-1.16	-5.47	-4.31 CaSO4
Aragonite	0.11	-8.11	-8.22 CaCO3
Artinite	-6.65	3.78	10.43 MgCO3:Mg(OH)2:3H2O
Birnessite	-14.51	3.58	18.09 MnO2
Bixbyite	-12.03	-11.81	0.21 Mn2O3
Brucite	-5.49	12.14	17.63 Mg(OH)2
Calcite	0.31	-8.11	-8.42 CaCO3
CaMoO4	-1.63	-9.56	-7.94 CaMoO4
CaSeO3:2H2O	-6.90	-3.95	2.95 CaSeO3:2H2O
CaSeO4:2H2O	-19.71	-22.67	-2.96 CaSeO4:2H2O
CH4(g)	-53.59	-96.41	-42.82 CH4
CO2(g)	-2.32	-20.49	-18.18 CO2
Dolomite(disordered)	-0.25	-16.47	-16.22 CaMg(CO3)2
Dolomite(ordered)	0.35	-16.47	-16.82 CaMg(CO3)2
Epsomite	-3.52	-5.72	-2.21 MgSO4:7H2O
Fe(OH)2	-3.58	9.98	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	5.79	2.75	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-6.25	-4.69	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-16.73	-37.36	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-39.87	-41.93	-2.06 Fe2(SO4)3
Fe3(OH)8	1.40	21.62	20.22 Fe3(OH)8
FeMoO4	-1.94	-11.96	-10.01 FeMoO4
Ferrihydrite	2.12	5.82	3.70 Fe(OH)3
Ferroselite	-8.94	-27.86	-18.92 FeSe2
FeSe	-7.41	-18.43	-11.01 FeSe
Goethite	4.91	5.82	0.91 FeOOH
Gummitite	-9.87	-1.64	8.23 UO3
Gypsum	-0.86	-5.47	-4.62 CaSO4:2H2O
H-Jarosite	-7.75	-18.26	-10.51 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-8.73	-21.94	-13.21 H2MoO4
H2Se(g)	-23.56	-28.41	-4.85 H2Se
Halite	-6.55	-4.98	1.58 NaCl
Hausmannite	-12.87	51.07	63.94 Mn3O4
Hematite	12.17	11.64	-0.53 Fe2O3

Huntite -3.96 -33.19 -29.22 CaMg3(CO3)4
 Hydromagnesite -14.04 -21.30 -7.26 Mg5(CO3)4(OH)2·4H2O
 K-Jarosite -0.74 -14.64 -13.90 KFe3(SO4)2(OH)6
 K2MoO4 -18.00 -14.72 3.29 K2MoO4
 K2SeO4 -27.09 -27.82 -0.73 K2SeO4
 Lepidocrocite 4.45 5.82 1.37 FeOOH
 Lime -21.66 12.38 34.04 CaO
 Maghemite 5.25 11.64 6.39 Fe2O3
 Magnesioferrite 4.99 23.77 18.78 Fe2MgO4
 Magnesite -0.76 -8.36 -7.60 MgCO3
 Magnetite 16.78 21.62 4.84 Fe3O4
 Manganite -5.15 20.19 25.34 MnOOH
 Melanterite -5.52 -7.87 -2.35 FeSO4·7H2O
 Mg(OH)2(active) -6.66 12.14 18.79 Mg(OH)2
 MgMoO4 -7.96 -9.81 -1.85 MgMoO4
 MgSeO3·6H2O -7.22 -4.20 3.02 MgSeO3·6H2O
 MgSeO4·6H2O -21.71 -22.91 -1.20 MgSeO4·6H2O
 Mirabilite -5.69 -7.36 -1.66 Na2SO4·10H2O
 Mn2(SO4)3 -60.80 -65.38 -4.58 Mn2(SO4)3
 MnCl2·4H2O -12.55 -9.76 2.79 MnCl2·4H2O
 MnSe -21.89 -17.72 4.18 MnSe
 MnSeO3 -6.77 -5.64 1.13 MnSeO3
 MnSeO3·2H2O -6.56 -5.64 0.92 MnSeO3·2H2O
 MnSeO4·5H2O -22.30 -24.35 -2.05 MnSeO4·5H2O
 MnSO4 -10.19 -7.16 3.03 MnSO4
 MoO3 -13.94 -21.94 -8.00 MoO3
 Na-Jarosite -2.85 -13.00 -10.16 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -16.40 -33.39 -16.98 Na2Mo2O7
 Na2MoO4 -13.00 -11.44 1.56 Na2MoO4
 Na2MoO4·2H2O -12.67 -11.44 1.22 Na2MoO4·2H2O
 Na2SeO3·5H2O -16.13 -5.83 10.30 Na2SeO3·5H2O
 Na2SeO4 -25.83 -24.55 1.28 Na2SeO4
 Natron -8.23 -9.99 -1.77 Na2CO3·10H2O
 Nesquehonite -3.86 -8.36 -4.50 MgCO3·3H2O
 Nsutite -13.92 3.58 17.50 MnO2
 O2(g) -49.07 37.96 87.03 O2
 Periclase -10.49 12.14 22.63 MgO
 Portlandite -11.31 12.38 23.69 Ca(OH)2
 Pyrochroite -5.17 10.70 15.86 Mn(OH)2
 Pyrolusite -13.58 29.68 43.26 MnO2
 Rhodochrosite 0.77 -9.80 -10.57 MnCO3
 Rutherfordine -7.65 -22.13 -14.48 UO2CO3
 Schoepite -7.98 -1.64 6.34 UO2(OH)2·H2O
 Semetal(am) -2.25 -9.43 -7.18 Se
 Semetal(hex) -1.61 -9.43 -7.82 Se
 SeO2 -16.45 -16.33 0.11 SeO2
 SeO3 -57.10 -35.05 22.05 SeO3
 Siderite -0.38 -10.51 -10.13 FeCO3
 Thenardite -7.74 -7.35 0.38 Na2SO4
 Thermonatrite -10.70 -9.99 0.71 Na2CO3·H2O
 U3O8 -17.70 6.73 24.43 U3O8
 U4O9 -22.58 -22.66 -0.07 U4O9
 UO2(am) -12.10 -10.41 1.69 UO2
 UO2(NO3)2 -41.36 -28.64 12.72 UO2(NO3)2
 UO2(NO3)2·2H2O -33.66 -28.64 5.03 UO2(NO3)2·2H2O
 UO2(NO3)2·3H2O -32.09 -28.64 3.45 UO2(NO3)2·3H2O
 UO2(NO3)2·6H2O -30.54 -28.64 1.90 UO2(NO3)2·6H2O
 UO2(OH)2(beta) -7.64 -1.64 6.00 UO2(OH)2
 UO2SeO4·4H2O -34.44 -36.69 -2.25 UO2SeO4·4H2O
 UO3 -9.90 -1.64 8.26 UO3
 Uraninite -6.28 -10.41 -4.13 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 3. SAG1-3

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

Elements	Molality	Moles
Alkalinity	3.481e-03	3.481e-03
Ca	4.247e-03	4.247e-03
Cl	2.581e-03	2.581e-03
Fe(2)	1.793e-05	1.793e-05
Fe(3)	5.379e-07	5.379e-07
K	1.247e-04	1.247e-04
Mg	2.080e-03	2.080e-03
Mn	1.387e-04	1.387e-04
Mo	3.663e-07	3.663e-07
N(-3)	4.139e-05	4.139e-05
N(5)	1.430e-06	1.430e-06
Na	5.357e-03	5.357e-03
O(0)	1.001e-05	1.001e-05
S(6)	6.556e-03	6.556e-03
Se	4.692e-09	4.692e-09
U	2.259e-08	2.259e-08

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

pH = 7.630
 pe = 1.700
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.576e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.634e-03
 Total CO2 (mol/kg) = 3.634e-03
 Temperature (°C) = 13.80
 Electrical balance (eq) = -6.846e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -2.17
 Iterations = 21 (48 overall)
 Total H = 1.110176e+02
 Total O = 5.554397e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	1.4700	0.0837
N(-3)/N(5)	5.8358	0.3323
O(-2)/O(0)	13.3668	0.7610

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	2.085e-07	1.783e-07	-6.681	-6.749	-0.068	(0)	
H+	2.725e-08	2.344e-08	-7.565	-7.630	-0.065	0.00	
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.03	
C(4)	3.634e-03						
HCO3-	3.318e-03	2.872e-03	-2.479	-2.542	-0.063	(0)	
H2CO3	1.749e-04	1.749e-04	-3.757	-3.757	0.000	(0)	
CaHCO3+	7.810e-05	6.785e-05	-4.107	-4.168	-0.061	(0)	
MgHCO3+	2.882e-05	2.474e-05	-4.540	-4.607	-0.066	(0)	
CaCO3	9.774e-06	9.774e-06	-5.010	-5.010	0.000	(0)	
NaHCO3	9.090e-06	9.090e-06	-5.041	-5.041	0.000	(0)	
CO3-2	8.335e-06	4.564e-06	-5.079	-5.341	-0.262	(0)	
MnHCO3+	3.335e-06	2.880e-06	-5.477	-5.541	-0.064	(0)	
MgCO3	2.817e-06	2.817e-06	-5.550	-5.550	0.000	(0)	
NaCO3-	6.132e-07	5.309e-07	-6.212	-6.275	-0.063	(0)	
FeHCO3+	2.167e-07	1.883e-07	-6.664	-6.725	-0.061	(0)	

Ca2UO2(CO3)3 1.696e-08 1.706e-08 -7.771 -7.768 0.003 (0)
 CaUO2(CO3)3-2 5.413e-09 2.964e-09 -8.267 -8.528 -0.262 (0)
 UO2(CO3)3-4 1.626e-10 8.421e-12 -9.789 -11.075 -1.286 (0)
 UO2(CO3)2-2 3.195e-11 1.524e-11 -10.495 -10.817 -0.321 (0)
 MgUO2(CO3)3-2 1.931e-11 1.058e-11 -10.714 -10.976 -0.262 (0)
 UO2CO3 2.022e-13 2.022e-13 -12.694 -12.694 0.000 (0)
 (UO2)2CO3(OH)3- 9.281e-18 7.984e-18 -17.032 -17.098 -0.065 (0)
 (UO2)3(CO3)6-6 1.107e-26 4.901e-29 -25.956 -28.310 -2.354 (0)

Ca 4.247e-03

Ca+2 3.174e-03 1.738e-03 -2.498 -2.760 -0.262 (0)
 CaSO4 9.851e-04 9.851e-04 -3.007 -3.007 0.000 (0)
 CaHCO3+ 7.810e-05 6.785e-05 -4.107 -4.168 -0.061 (0)
 CaCO3 9.774e-06 9.774e-06 -5.010 -5.010 0.000 (0)
 Ca2UO2(CO3)3 1.696e-08 1.706e-08 -7.771 -7.768 0.003 (0)
 CaNO3+ 8.800e-09 7.314e-09 -8.055 -8.136 -0.080 (0)
 CaOH+ 6.247e-09 5.427e-09 -8.204 -8.265 -0.061 (0)
 CaUO2(CO3)3-2 5.413e-09 2.964e-09 -8.267 -8.528 -0.262 (0)
 CaNH3+2 3.776e-09 1.801e-09 -8.423 -8.744 -0.321 (0)
 Ca(NH3)2+2 1.237e-15 5.903e-16 -14.907 -15.229 -0.321 (0)

Cl 2.581e-03

Cl- 2.581e-03 2.220e-03 -2.588 -2.654 -0.065 (0)
 MnCl+ 1.732e-07 1.496e-07 -6.761 -6.825 -0.064 (0)
 MnCl2 4.692e-10 4.692e-10 -9.329 -9.329 0.000 (0)
 MnCl3- 3.322e-13 2.869e-13 -12.479 -12.542 -0.064 (0)
 FeCl+2 7.696e-19 4.281e-19 -18.114 -18.368 -0.255 (0)
 UO2Cl+ 3.991e-20 3.317e-20 -19.399 -19.479 -0.080 (0)
 FeCl2+ 7.062e-21 6.099e-21 -20.151 -20.215 -0.064 (0)
 UO2Cl2 4.352e-24 4.378e-24 -23.361 -23.359 0.003 (0)
 FeCl3 1.354e-24 1.354e-24 -23.868 -23.868 0.000 (0)
 UCl+3 0.000e+00 0.000e+00 -40.738 -41.461 -0.723 (0)

Fe(2) 1.793e-05

Fe+2 1.374e-05 6.552e-06 -4.862 -5.184 -0.321 (0)
 FeSO4 3.923e-06 3.923e-06 -5.406 -5.406 0.000 (0)
 FeHCO3+ 2.167e-07 1.883e-07 -6.664 -6.725 -0.061 (0)
 FeOH+ 5.386e-08 4.651e-08 -7.269 -7.332 -0.064 (0)
 Fe(OH)2 5.809e-12 5.809e-12 -11.236 -11.236 0.000 (0)
 Fe(OH)3- 8.204e-13 7.085e-13 -12.086 -12.150 -0.064 (0)

Fe(3) 5.379e-07

Fe(OH)2+ 4.906e-07 4.247e-07 -6.309 -6.372 -0.063 (0)
 Fe(OH)3 3.821e-08 3.821e-08 -7.418 -7.418 0.000 (0)
 Fe(OH)4- 9.045e-09 7.830e-09 -8.044 -8.106 -0.063 (0)
 FeOH+2 2.366e-12 1.316e-12 -11.626 -11.881 -0.255 (0)
 FeSO4+ 2.224e-16 1.921e-16 -15.653 -15.717 -0.064 (0)
 Fe+3 3.555e-17 9.171e-18 -16.449 -17.038 -0.588 (0)
 Fe(SO4)2- 1.498e-17 1.245e-17 -16.825 -16.905 -0.080 (0)
 FeCl+2 7.696e-19 4.281e-19 -18.114 -18.368 -0.255 (0)
 FeCl2+ 7.062e-21 6.099e-21 -20.151 -20.215 -0.064 (0)
 Fe2(OH)2+4 1.669e-21 8.640e-23 -20.778 -22.063 -1.286 (0)
 FeNO3+2 4.208e-22 2.007e-22 -21.376 -21.697 -0.321 (0)
 FeHSeO3+2 1.049e-22 5.006e-23 -21.979 -22.301 -0.321 (0)
 FeCl3 1.354e-24 1.354e-24 -23.868 -23.868 0.000 (0)
 Fe3(OH)4+5 4.805e-26 4.705e-28 -25.318 -27.327 -2.009 (0)

H(0) 3.458e-22

H2 1.729e-22 1.739e-22 -21.762 -21.760 0.003 (0)

K 1.247e-04

K+ 1.225e-04 1.054e-04 -3.912 -3.977 -0.065 (0)
 KSO4- 2.235e-06 1.935e-06 -5.651 -5.713 -0.063 (0)

Mg 2.080e-03

Mg+2 1.637e-03 8.963e-04 -2.786 -3.048 -0.262 (0)
 MgSO4 4.118e-04 4.118e-04 -3.385 -3.385 0.000 (0)
 MgHCO3+ 2.882e-05 2.474e-05 -4.540 -4.607 -0.066 (0)
 MgCO3 2.817e-06 2.817e-06 -5.550 -5.550 0.000 (0)
 MgOH+ 6.047e-08 5.268e-08 -7.218 -7.278 -0.060 (0)
 MgUO2(CO3)3-2 1.931e-11 1.058e-11 -10.714 -10.976 -0.262 (0)

Mn(2) 1.387e-04

Mn+2 1.122e-04 5.352e-05 -3.950 -4.271 -0.321 (0)

MnSO4	2.296e-05	2.296e-05	-4.639	-4.639	0.000	(0)
MnHCO3+	3.335e-06	2.880e-06	-5.477	-5.541	-0.064	(0)
MnCl+	1.732e-07	1.496e-07	-6.761	-6.825	-0.064	(0)
MnOH+	2.776e-08	2.397e-08	-7.557	-7.620	-0.064	(0)
MnCl2	4.692e-10	4.692e-10	-9.329	-9.329	0.000	(0)
MnNO3+	1.247e-10	1.037e-10	-9.904	-9.984	-0.080	(0)
MnCl3-	3.322e-13	2.869e-13	-12.479	-12.542	-0.064	(0)
Mn(NO3)2	3.267e-16	3.267e-16	-15.486	-15.486	0.000	(0)
Mn(OH)3-	7.615e-17	6.577e-17	-16.118	-16.182	-0.064	(0)
MnSe	2.188e-22	2.188e-22	-21.660	-21.660	0.000	(0)
Mn(OH)4-2	1.639e-22	9.117e-23	-21.785	-22.040	-0.255	(0)
MnSeO4	1.428e-22	1.428e-22	-21.845	-21.845	0.000	(0)
Mn(3)	8.509e-29					
Mn+3	8.509e-29	2.195e-29	-28.070	-28.659	-0.588	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-59.462	-59.716	-0.255	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-68.082	-68.151	-0.069	(0)
Mo	3.663e-07					
MoO4-2	3.662e-07	2.005e-07	-6.436	-6.698	-0.262	(0)
HMoO4-	8.215e-11	6.828e-11	-10.085	-10.166	-0.080	(0)
H2MoO4	2.419e-14	2.419e-14	-13.616	-13.616	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-50.482	-53.375	-2.893	(0)
HMo7O24-5	0.000e+00	0.000e+00	-52.677	-54.686	-2.009	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-56.269	-57.555	-1.286	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-61.202	-61.925	-0.723	(0)
N(-3)	4.139e-05					
NH4+	3.986e-05	3.384e-05	-4.399	-4.471	-0.071	(0)
NH4SO4-	1.162e-06	1.003e-06	-5.935	-5.999	-0.064	(0)
NH3	3.630e-07	3.630e-07	-6.440	-6.440	0.000	(0)
CaNH3+2	3.776e-09	1.801e-09	-8.423	-8.744	-0.321	(0)
Ca(NH3)2+2	1.237e-15	5.903e-16	-14.907	-15.229	-0.321	(0)
N(5)	1.430e-06					
NO3-	1.421e-06	1.222e-06	-5.847	-5.913	-0.065	(0)
CaNO3+	8.800e-09	7.314e-09	-8.055	-8.136	-0.080	(0)
MnNO3+	1.247e-10	1.037e-10	-9.904	-9.984	-0.080	(0)
Mn(NO3)2	3.267e-16	3.267e-16	-15.486	-15.486	0.000	(0)
FeNO3+2	4.208e-22	2.007e-22	-21.376	-21.697	-0.321	(0)
UO2NO3+	4.200e-23	3.491e-23	-22.377	-22.457	-0.080	(0)
Na	5.357e-03					
Na+	5.271e-03	4.534e-03	-2.278	-2.344	-0.065	(0)
NaSO4-	7.659e-05	6.631e-05	-4.116	-4.178	-0.063	(0)
NaHCO3	9.090e-06	9.090e-06	-5.041	-5.041	0.000	(0)
NaCO3-	6.132e-07	5.309e-07	-6.212	-6.275	-0.063	(0)
O(0)	1.001e-05					
O2	5.006e-06	5.036e-06	-5.300	-5.298	0.003	(0)
S(6)	6.556e-03					
SO4-2	5.052e-03	2.766e-03	-2.297	-2.558	-0.262	(0)
CaSO4	9.851e-04	9.851e-04	-3.007	-3.007	0.000	(0)
MgSO4	4.118e-04	4.118e-04	-3.385	-3.385	0.000	(0)
NaSO4-	7.659e-05	6.631e-05	-4.116	-4.178	-0.063	(0)
MnSO4	2.296e-05	2.296e-05	-4.639	-4.639	0.000	(0)
FeSO4	3.923e-06	3.923e-06	-5.406	-5.406	0.000	(0)
KSO4-	2.235e-06	1.935e-06	-5.651	-5.713	-0.063	(0)
NH4SO4-	1.162e-06	1.003e-06	-5.935	-5.999	-0.064	(0)
HSO4-	5.206e-09	4.482e-09	-8.283	-8.349	-0.065	(0)
FeSO4+	2.224e-16	1.921e-16	-15.653	-15.717	-0.064	(0)
UO2SO4	3.621e-17	3.621e-17	-16.441	-16.441	0.000	(0)
Fe(SO4)2-	1.498e-17	1.245e-17	-16.825	-16.905	-0.080	(0)
UO2(SO4)2-2	2.085e-18	9.948e-19	-17.681	-18.002	-0.321	(0)
U(SO4)2	3.263e-36	3.263e-36	-35.486	-35.486	0.000	(0)
USO4+2	4.614e-37	2.201e-37	-36.336	-36.657	-0.321	(0)
Se(-2)	2.821e-20					
HSe-	2.798e-20	2.326e-20	-19.553	-19.633	-0.080	(0)
MnSe	2.188e-22	2.188e-22	-21.660	-21.660	0.000	(0)
H2Se	4.017e-24	4.017e-24	-23.396	-23.396	0.000	(0)

Se-2 9.750e-28 4.651e-28 -27.011 -27.332 -0.321 (0)
 Se(4) 4.692e-09
 HSeO3- 3.684e-09 3.062e-09 -8.434 -8.514 -0.080 (0)
 SeO3-2 1.007e-09 4.805e-10 -8.997 -9.318 -0.321 (0)
 H2SeO3 2.777e-14 2.777e-14 -13.556 -13.556 0.000 (0)
 FeHSeO3+2 1.049e-22 5.006e-23 -21.979 -22.301 -0.321 (0)
 Se(6) 2.272e-20
 SeO4-2 2.257e-20 1.236e-20 -19.646 -19.908 -0.262 (0)
 MnSeO4 1.428e-22 1.428e-22 -21.845 -21.845 0.000 (0)
 HSeO4- 1.217e-26 1.011e-26 -25.915 -25.995 -0.080 (0)
 U(3) 0.000e+00
 U+3 0.000e+00 0.000e+00 -51.115 -51.839 -0.723 (0)
 U(4) 4.747e-17
 U(OH)5- 4.742e-17 3.941e-17 -16.324 -16.404 -0.080 (0)
 U(OH)4 4.659e-20 4.659e-20 -19.332 -19.332 0.000 (0)
 U(OH)3+ 5.526e-24 4.592e-24 -23.258 -23.338 -0.080 (0)
 U(OH)2+2 1.443e-28 6.883e-29 -27.841 -28.162 -0.321 (0)
 UOH+3 6.090e-34 1.152e-34 -33.215 -33.939 -0.723 (0)
 U(SO4)2 3.263e-36 3.263e-36 -35.486 -35.486 0.000 (0)
 USO4+2 4.614e-37 2.201e-37 -36.336 -36.657 -0.321 (0)
 U+4 4.378e-40 0.000e+00 -39.359 -40.645 -1.286 (0)
 UCl+3 0.000e+00 0.000e+00 -40.738 -41.461 -0.723 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -140.065 -146.575 -6.510 (0)
 U(5) 2.155e-16
 UO2+ 2.155e-16 1.791e-16 -15.667 -15.747 -0.080 (0)
 U(6) 2.259e-08
 Ca2UO2(CO3)3 1.696e-08 1.706e-08 -7.771 -7.768 0.003 (0)
 CaUO2(CO3)3-2 5.413e-09 2.964e-09 -8.267 -8.528 -0.262 (0)
 UO2(CO3)3-4 1.626e-10 8.421e-12 -9.789 -11.075 -1.286 (0)
 UO2(CO3)2-2 3.195e-11 1.524e-11 -10.495 -10.817 -0.321 (0)
 MgUO2(CO3)3-2 1.931e-11 1.058e-11 -10.714 -10.976 -0.262 (0)
 UO2(OH)2 1.038e-12 1.044e-12 -11.984 -11.981 0.003 (0)
 UO2CO3 2.022e-13 2.022e-13 -12.694 -12.694 0.000 (0)
 UO2(OH)3- 6.409e-14 5.513e-14 -13.193 -13.259 -0.065 (0)
 UO2OH+ 3.631e-16 3.017e-16 -15.440 -15.520 -0.080 (0)
 UO2SO4 3.621e-17 3.621e-17 -16.441 -16.441 0.000 (0)
 UO2+2 2.164e-17 1.185e-17 -16.665 -16.926 -0.262 (0)
 (UO2)2CO3(OH)3- 9.281e-18 7.984e-18 -17.032 -17.098 -0.065 (0)
 UO2(SO4)2-2 2.085e-18 9.948e-19 -17.681 -18.002 -0.321 (0)
 UO2(OH)4-2 6.691e-20 3.664e-20 -19.175 -19.436 -0.262 (0)
 UO2Cl+ 3.991e-20 3.317e-20 -19.399 -19.479 -0.080 (0)
 UO2NO3+ 4.200e-23 3.491e-23 -22.377 -22.457 -0.080 (0)
 UO2Cl2 4.352e-24 4.378e-24 -23.361 -23.359 0.003 (0)
 (UO2)2(OH)2+2 7.389e-25 3.525e-25 -24.131 -24.453 -0.321 (0)
 (UO2)3(CO3)6-6 1.107e-26 4.901e-29 -25.956 -28.310 -2.354 (0)
 (UO2)2OH+3 4.555e-29 1.175e-29 -28.341 -28.930 -0.588 (0)
 (UO2)3(OH)7- 4.411e-29 3.794e-29 -28.355 -28.421 -0.065 (0)
 (UO2)3(OH)5+ 1.339e-29 1.113e-29 -28.873 -28.954 -0.080 (0)
 (UO2)3(OH)4+2 1.183e-32 6.478e-33 -31.927 -32.189 -0.262 (0)
 (UO2)4(OH)7+ 6.580e-37 5.661e-37 -36.182 -36.247 -0.065 (0)

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

Phase SI** log IAP log K(286 K, 1 atm)

(NH4)2SeO4 -29.30 -28.85 0.45 (NH4)2SeO4
 Anhydrite -1.01 -5.32 -4.31 CaSO4
 Aragonite 0.12 -8.10 -8.22 CaCO3
 Artinite -6.60 3.82 10.42 MgCO3:Mg(OH)2:3H2O
 Birnessite -14.53 3.56 18.09 MnO2
 Bixbyite -11.74 -11.54 0.21 Mn2O3
 Brucite -5.41 12.21 17.62 Mg(OH)2
 Calcite 0.32 -8.10 -8.43 CaCO3
 CaMoO4 -1.52 -9.46 -7.94 CaMoO4
 CaSeO3:2H2O -6.59 -3.64 2.95 CaSeO3:2H2O
 CaSeO4:2H2O -19.70 -22.67 -2.96 CaSeO4:2H2O

CH4(g) -52.44 -95.24 -42.80 CH4
 CO2(g) -2.43 -20.60 -18.17 CO2
 Dolomite(disordered) -0.27 -16.49 -16.22 CaMg(CO3)2
 Dolomite(ordered) 0.33 -16.49 -16.82 CaMg(CO3)2
 Epsomite -3.40 -5.61 -2.21 MgSO4:7H2O
 Fe(OH)2 -3.49 10.08 13.56 Fe(OH)2
 Fe(OH)2.7Cl.3 5.81 2.77 -3.04 Fe(OH)2.7Cl.3
 Fe2(OH)4SeO3 -5.99 -4.44 1.55 Fe2(OH)4SeO3
 Fe2(SeO3)3:2H2O -16.10 -36.73 -20.63 Fe2(SeO3)3:2H2O
 Fe2(SO4)3 -39.67 -41.75 -2.08 Fe2(SO4)3
 Fe3(OH)8 1.56 21.78 20.22 Fe3(OH)8
 FeMoO4 -1.87 -11.88 -10.02 FeMoO4
 Ferrihydrite 2.16 5.85 3.69 Fe(OH)3
 Ferroselite -6.87 -25.79 -18.92 FeSe2
 FeSe -6.17 -17.19 -11.01 FeSe
 Goethite 4.95 5.85 0.91 FeOOH
 Gummite -9.89 -1.67 8.23 UO3
 Gypsum -0.70 -5.32 -4.62 CaSO4:2H2O
 H-Jarosite -7.56 -18.08 -10.52 (H3O)Fe3(SO4)2(OH)6
 H2MoO4 -8.75 -21.96 -13.21 H2MoO4
 H2Se(g) -22.41 -27.26 -4.86 H2Se
 Halite -6.57 -5.00 1.58 NaCl
 Hausmannite -12.28 51.62 63.91 Mn3O4
 Hematite 12.24 11.70 -0.54 Fe2O3
 Huntite -4.03 -33.27 -29.23 CaMg3(CO3)4
 Hydromagnesite -14.07 -21.34 -7.27 Mg5(CO3)4(OH)2:4H2O
 K-Jarosite -0.52 -14.43 -13.91 KFe3(SO4)2(OH)6
 K2MoO4 -17.94 -14.65 3.29 K2MoO4
 K2SeO4 -27.13 -27.86 -0.73 K2SeO4
 Lepidocrocite 4.48 5.85 1.37 FeOOH
 Lime -21.53 12.50 34.03 CaO
 Maghemite 5.32 11.70 6.39 Fe2O3
 Magnesioferrite 5.15 23.92 18.77 Fe2MgO4
 Magnesite -0.79 -8.39 -7.60 MgCO3
 Magnetite 16.95 21.78 4.83 Fe3O4
 Manganite -5.02 20.32 25.34 MnOOH
 Melanterite -5.39 -7.74 -2.35 FeSO4:7H2O
 Mg(OH)2(active) -6.58 12.21 18.79 Mg(OH)2
 MgMoO4 -7.90 -9.75 -1.85 MgMoO4
 MgSeO3:6H2O -6.95 -3.93 3.02 MgSeO3:6H2O
 MgSeO4:6H2O -21.76 -22.96 -1.20 MgSeO4:6H2O
 Mirabilite -5.59 -7.25 -1.66 Na2SO4:10H2O
 Mn2(SO4)3 -60.40 -64.99 -4.59 Mn2(SO4)3
 MnCl2:4H2O -12.37 -9.58 2.79 MnCl2:4H2O
 MnSe -20.45 -16.27 4.17 MnSe
 MnSeO3 -6.29 -5.16 1.13 MnSeO3
 MnSeO3:2H2O -6.08 -5.16 0.92 MnSeO3:2H2O
 MnSeO4:5H2O -22.13 -24.18 -2.05 MnSeO4:5H2O
 MnSO4 -9.86 -6.83 3.03 MnSO4
 MoO3 -13.96 -21.96 -8.00 MoO3
 Na-Jarosite -2.63 -12.79 -10.16 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -16.36 -33.34 -16.98 Na2Mo2O7
 Na2MoO4 -12.94 -11.38 1.56 Na2MoO4
 Na2MoO4:2H2O -12.61 -11.39 1.22 Na2MoO4:2H2O
 Na2SeO3:5H2O -15.87 -5.57 10.30 Na2SeO3:5H2O
 Na2SeO4 -25.87 -24.59 1.28 Na2SeO4
 Natron -8.27 -10.03 -1.76 Na2CO3:10H2O
 Nesquehonite -3.88 -8.39 -4.50 MgCO3:3H2O
 Nsutite -13.94 3.56 17.50 MnO2
 O2(g) -49.68 37.32 87.00 O2
 Periclase -10.41 12.21 22.62 MgO
 Portlandite -11.18 12.50 23.68 Ca(OH)2
 Pyrochroite -4.87 10.99 15.86 Mn(OH)2
 Pyrolusite -13.59 29.65 43.24 MnO2
 Rhodochrosite 0.96 -9.61 -10.57 MnCO3
 Rutherfordine -7.79 -22.27 -14.48 UO2CO3

Schoepite -8.00 -1.67 6.33 UO₂(OH)₂:H₂O
 Semetal(am) -1.42 -8.60 -7.18 Se
 Semetal(hex) -0.79 -8.60 -7.82 Se
 SeO₂ -16.26 -16.14 0.12 SeO₂
 SeO₃ -57.21 -35.17 22.04 SeO₃
 Siderite -0.39 -10.52 -10.13 FeCO₃
 Thenardite -7.63 -7.25 0.38 Na₂SO₄
 Thermonatrite -10.74 -10.03 0.71 Na₂CO₃:H₂O
 U₃O₈ -17.46 6.94 24.40 U₃O₈
 U₄O₉ -21.74 -21.84 -0.10 U₄O₉
 UO₂(am) -11.81 -10.12 1.68 UO₂
 UO₂(NO₃)₂ -41.47 -28.75 12.72 UO₂(NO₃)₂
 UO₂(NO₃)₂:2H₂O -33.78 -28.75 5.02 UO₂(NO₃)₂:2H₂O
 UO₂(NO₃)₂:3H₂O -32.21 -28.75 3.45 UO₂(NO₃)₂:3H₂O
 UO₂(NO₃)₂:6H₂O -30.66 -28.75 1.90 UO₂(NO₃)₂:6H₂O
 UO₂(OH)₂(beta) -7.67 -1.67 6.00 UO₂(OH)₂
 UO₂SeO₄:4H₂O -34.58 -36.83 -2.25 UO₂SeO₄:4H₂O
 UO₃ -9.92 -1.67 8.25 UO₃
 Uraninite -5.99 -10.12 -4.14 UO₂

**For a gas, SI = log₁₀(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 4. SAG1-4

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

Elements	Molality	Moles
Alkalinity	2.963e-03	2.963e-03
Ca	8.298e-03	8.298e-03
Cl	1.139e-03	1.139e-03
Fe(2)	4.861e-05	4.861e-05
Fe(3)	1.345e-05	1.345e-05
K	9.326e-05	9.326e-05
Mg	2.526e-03	2.526e-03
Mn	3.884e-05	3.884e-05
Mo	9.042e-08	9.042e-08
N(-3)	1.137e-05	1.137e-05
N(5)	1.430e-06	1.430e-06
Na	3.246e-03	3.246e-03
O(0)	6.887e-06	6.887e-06
S(6)	1.116e-02	1.116e-02
Se	2.537e-09	2.537e-09
U	8.459e-09	8.459e-09

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

pH = 7.480
 pe = 0.900
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 3.516e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.152e-03
 Total CO₂ (mol/kg) = 3.152e-03
 Temperature (°C) = 12.70
 Electrical balance (eq) = -1.229e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -3.16
 Iterations = 20 (68 overall)
 Total H = 1.110171e+02
 Total O = 5.556096e+01

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

Redox couple	pe Eh (volts)
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Fe(2)/Fe(3)	2.8516	0.1617
N(-3)/N(5)	6.1626	0.3495
O(-2)/O(0)	13.5606	0.7691

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

Species	Log Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.378e-07	1.154e-07	-6.861	-6.938	-0.077	(0)	
H+	3.923e-08	3.311e-08	-7.406	-7.480	-0.074	0.00	
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.03	
C(4)	3.152e-03						
HCO3-	2.791e-03	2.373e-03	-2.554	-2.625	-0.070	(0)	
H2CO3	2.072e-04	2.072e-04	-3.684	-3.684	0.000	(0)	
CaHCO3+	1.070e-04	9.141e-05	-3.970	-4.039	-0.069	(0)	
MgHCO3+	2.550e-05	2.144e-05	-4.593	-4.669	-0.075	(0)	
CaCO3	9.164e-06	9.164e-06	-5.038	-5.038	0.000	(0)	
CO3-2	5.139e-06	2.608e-06	-5.289	-5.584	-0.295	(0)	
NaHCO3	4.536e-06	4.536e-06	-5.343	-5.343	0.000	(0)	
MgCO3	1.667e-06	1.667e-06	-5.778	-5.778	0.000	(0)	
MnHCO3+	6.641e-07	5.630e-07	-6.178	-6.250	-0.072	(0)	
FeHCO3+	4.032e-07	3.443e-07	-6.394	-6.463	-0.069	(0)	
NaCO3-	2.178e-07	1.852e-07	-6.662	-6.732	-0.070	(0)	
Ca2UO2(CO3)3	6.975e-09	7.032e-09	-8.156	-8.153	0.004	(0)	
CaUO2(CO3)3-2	1.430e-09	7.254e-10	-8.845	-9.139	-0.295	(0)	
UO2(CO3)3-4	4.126e-11	1.305e-12	-10.384	-11.884	-1.500	(0)	
UO2(CO3)2-2	8.959e-12	3.778e-12	-11.048	-11.423	-0.375	(0)	
MgUO2(CO3)3-2	3.198e-12	1.623e-12	-11.495	-11.790	-0.295	(0)	
UO2CO3	8.944e-14	8.944e-14	-13.048	-13.048	0.000	(0)	
(UO2)2CO3(OH)3-	1.192e-18	1.006e-18	-17.924	-17.997	-0.074	(0)	
(UO2)3(CO3)6-6	4.168e-28	9.289e-31	-27.380	-30.032	-2.652	(0)	
Ca	8.298e-03						
Ca+2	5.770e-03	2.927e-03	-2.239	-2.534	-0.295	(0)	
CaSO4	2.412e-03	2.412e-03	-2.618	-2.618	0.000	(0)	
CaHCO3+	1.070e-04	9.141e-05	-3.970	-4.039	-0.069	(0)	
CaCO3	9.164e-06	9.164e-06	-5.038	-5.038	0.000	(0)	
CaNO3+	1.507e-08	1.214e-08	-7.822	-7.916	-0.094	(0)	
Ca2UO2(CO3)3	6.975e-09	7.032e-09	-8.156	-8.153	0.004	(0)	
CaOH+	6.832e-09	5.835e-09	-8.165	-8.234	-0.069	(0)	
CaUO2(CO3)3-2	1.430e-09	7.254e-10	-8.845	-9.139	-0.295	(0)	
CaNH3+2	1.353e-09	5.707e-10	-8.869	-9.244	-0.375	(0)	
Ca(NH3)2+2	8.342e-17	3.518e-17	-16.079	-16.454	-0.375	(0)	
Cl	1.139e-03						
Cl-	1.139e-03	9.610e-04	-2.944	-3.017	-0.074	(0)	
MnCl+	1.819e-08	1.542e-08	-7.740	-7.812	-0.072	(0)	
MnCl2	2.093e-11	2.093e-11	-10.679	-10.679	0.000	(0)	
MnCl3-	6.536e-15	5.540e-15	-14.185	-14.256	-0.072	(0)	
FeCl+2	1.762e-17	9.096e-18	-16.754	-17.041	-0.287	(0)	
FeCl2+	6.866e-20	5.820e-20	-19.163	-19.235	-0.072	(0)	
UO2Cl+	1.353e-20	1.090e-20	-19.869	-19.962	-0.094	(0)	
FeCl3	5.594e-24	5.594e-24	-23.252	-23.252	0.000	(0)	
UO2Cl2	6.340e-25	6.392e-25	-24.198	-24.194	0.004	(0)	
UCl+3	1.680e-39	2.408e-40	-38.775	-39.618	-0.844	(0)	
Fe(2)	4.861e-05						
Fe+2	3.522e-05	1.485e-05	-4.453	-4.828	-0.375	(0)	
FeSO4	1.291e-05	1.291e-05	-4.889	-4.889	0.000	(0)	
FeHCO3+	4.032e-07	3.443e-07	-6.394	-6.463	-0.069	(0)	
FeOH+	8.047e-08	6.821e-08	-7.094	-7.166	-0.072	(0)	
Fe(OH)2	5.441e-12	5.441e-12	-11.264	-11.264	0.000	(0)	
Fe(OH)3-	5.481e-13	4.646e-13	-12.261	-12.333	-0.072	(0)	
Fe(3)	1.345e-05						
Fe(OH)2+	1.275e-05	1.084e-05	-4.894	-4.965	-0.070	(0)	
Fe(OH)3	5.840e-07	5.840e-07	-6.234	-6.234	0.000	(0)	
Fe(OH)4-	1.178e-07	1.002e-07	-6.929	-6.999	-0.070	(0)	
FeOH+2	8.594e-11	4.437e-11	-10.066	-10.353	-0.287	(0)	

FeSO4+ 1.630e-14 1.382e-14 -13.788 -13.859 -0.072 (0)
 Fe+3 2.150e-15 4.672e-16 -14.668 -15.331 -0.663 (0)
 Fe(SO4)2- 1.650e-15 1.330e-15 -14.782 -14.876 -0.094 (0)
 FeCl+2 1.762e-17 9.096e-18 -16.754 -17.041 -0.287 (0)
 Fe2(OH)2+4 3.237e-18 1.024e-19 -17.490 -18.990 -1.500 (0)
 FeCl2+ 6.866e-20 5.820e-20 -19.163 -19.235 -0.072 (0)
 FeNO3+2 2.515e-20 1.061e-20 -19.599 -19.974 -0.375 (0)
 FeHSeO3+2 3.204e-21 1.351e-21 -20.494 -20.869 -0.375 (0)
 Fe3(OH)4+5 3.101e-21 1.406e-23 -20.509 -22.852 -2.344 (0)
 FeCl3 5.594e-24 5.594e-24 -23.252 -23.252 0.000 (0)
 H(0) 2.773e-20
 H2 1.387e-20 1.398e-20 -19.858 -19.855 0.004 (0)
 K 9.326e-05
 K+ 9.084e-05 7.667e-05 -4.042 -4.115 -0.074 (0)
 KSO4- 2.419e-06 2.057e-06 -5.616 -5.687 -0.070 (0)
 Mg 2.526e-03
 Mg+2 1.866e-03 9.465e-04 -2.729 -3.024 -0.295 (0)
 MgSO4 6.338e-04 6.338e-04 -3.198 -3.198 0.000 (0)
 MgHCO3+ 2.550e-05 2.144e-05 -4.593 -4.669 -0.075 (0)
 MgCO3 1.667e-06 1.667e-06 -5.778 -5.778 0.000 (0)
 MgOH+ 4.119e-08 3.530e-08 -7.385 -7.452 -0.067 (0)
 MgUO2(CO3)3-2 3.198e-12 1.623e-12 -11.495 -11.790 -0.295 (0)
 Mn(2) 3.884e-05
 Mn+2 3.022e-05 1.275e-05 -4.520 -4.895 -0.375 (0)
 MnSO4 7.930e-06 7.930e-06 -5.101 -5.101 0.000 (0)
 MnHCO3+ 6.641e-07 5.630e-07 -6.178 -6.250 -0.072 (0)
 MnCl+ 1.819e-08 1.542e-08 -7.740 -7.812 -0.072 (0)
 MnOH+ 4.357e-09 3.694e-09 -8.361 -8.433 -0.072 (0)
 MnNO3+ 2.994e-11 2.413e-11 -10.524 -10.617 -0.094 (0)
 MnCl2 2.093e-11 2.093e-11 -10.679 -10.679 0.000 (0)
 MnCl3- 6.536e-15 5.540e-15 -14.185 -14.256 -0.072 (0)
 Mn(NO3)2 7.451e-17 7.451e-17 -16.128 -16.128 0.000 (0)
 MnSe 1.020e-17 1.020e-17 -16.991 -16.991 0.000 (0)
 Mn(OH)3- 6.554e-18 5.556e-18 -17.183 -17.255 -0.072 (0)
 Mn(OH)4-2 1.056e-23 5.452e-24 -22.976 -23.263 -0.287 (0)
 MnSeO4 1.182e-25 1.182e-25 -24.927 -24.927 0.000 (0)
 Mn(3) 3.204e-30
 Mn+3 3.204e-30 6.962e-31 -29.494 -30.157 -0.663 (0)
 Mn(6) 0.000e+00
 MnO4-2 0.000e+00 0.000e+00 -64.951 -65.238 -0.287 (0)
 Mn(7) 0.000e+00
 MnO4- 0.000e+00 0.000e+00 -74.472 -74.551 -0.079 (0)
 Mo 9.042e-08
 MoO4-2 9.040e-08 4.586e-08 -7.044 -7.339 -0.295 (0)
 HMoO4- 2.650e-11 2.136e-11 -10.577 -10.670 -0.094 (0)
 H2MoO4 1.151e-14 1.151e-14 -13.939 -13.939 0.000 (0)
 Mo7O24-6 0.000e+00 0.000e+00 -53.125 -56.500 -3.375 (0)
 HMo7O24-5 0.000e+00 0.000e+00 -55.325 -57.669 -2.344 (0)
 H2Mo7O24-4 0.000e+00 0.000e+00 -58.889 -60.389 -1.500 (0)
 H3Mo7O24-3 0.000e+00 0.000e+00 -63.764 -64.608 -0.844 (0)
 N(-3) 1.137e-05
 NH4+ 1.084e-05 8.993e-06 -4.965 -5.046 -0.081 (0)
 NH4SO4- 4.626e-07 3.921e-07 -6.335 -6.407 -0.072 (0)
 NH3 6.280e-08 6.280e-08 -7.202 -7.202 0.000 (0)
 CaNH3+2 1.353e-09 5.707e-10 -8.869 -9.244 -0.375 (0)
 Ca(NH3)2+2 8.342e-17 3.518e-17 -16.079 -16.454 -0.375 (0)
 N(5) 1.430e-06
 NO3- 1.415e-06 1.194e-06 -5.849 -5.923 -0.074 (0)
 CaNO3+ 1.507e-08 1.214e-08 -7.822 -7.916 -0.094 (0)
 MnNO3+ 2.994e-11 2.413e-11 -10.524 -10.617 -0.094 (0)
 Mn(NO3)2 7.451e-17 7.451e-17 -16.128 -16.128 0.000 (0)
 FeNO3+2 2.515e-20 1.061e-20 -19.599 -19.974 -0.375 (0)
 UO2NO3+ 3.364e-23 2.711e-23 -22.473 -22.567 -0.094 (0)
 Na 3.246e-03
 Na+ 3.174e-03 2.679e-03 -2.498 -2.572 -0.074 (0)
 NaSO4- 6.766e-05 5.753e-05 -4.170 -4.240 -0.070 (0)

NaHCO3	4.536e-06	4.536e-06	-5.343	-5.343	0.000	(0)
NaCO3-	2.178e-07	1.852e-07	-6.662	-6.732	-0.070	(0)
O(0)	6.887e-06					
O2	3.443e-06	3.471e-06	-5.463	-5.459	0.004	(0)
S(6)	1.116e-02					
SO4-2	8.020e-03	4.069e-03	-2.096	-2.390	-0.295	(0)
CaSO4	2.412e-03	2.412e-03	-2.618	-2.618	0.000	(0)
MgSO4	6.338e-04	6.338e-04	-3.198	-3.198	0.000	(0)
NaSO4-	6.766e-05	5.753e-05	-4.170	-4.240	-0.070	(0)
FeSO4	1.291e-05	1.291e-05	-4.889	-4.889	0.000	(0)
MnSO4	7.930e-06	7.930e-06	-5.101	-5.101	0.000	(0)
KSO4-	2.419e-06	2.057e-06	-5.616	-5.687	-0.070	(0)
NH4SO4-	4.626e-07	3.921e-07	-6.335	-6.407	-0.072	(0)
HSO4-	1.065e-08	8.988e-09	-7.973	-8.046	-0.073	(0)
FeSO4+	1.630e-14	1.382e-14	-13.788	-13.859	-0.072	(0)
Fe(SO4)2-	1.650e-15	1.330e-15	-14.782	-14.876	-0.094	(0)
UO2SO4	4.020e-17	4.020e-17	-16.396	-16.396	0.000	(0)
UO2(SO4)2-2	3.741e-18	1.578e-18	-17.427	-17.802	-0.375	(0)
U(SO4)2	1.043e-33	1.043e-33	-32.982	-32.982	0.000	(0)
USO4+2	1.181e-34	4.981e-35	-33.928	-34.303	-0.375	(0)
Se(-2)	7.991e-15					
HSe-	7.979e-15	6.430e-15	-14.098	-14.192	-0.094	(0)
MnSe	1.020e-17	1.020e-17	-16.991	-16.991	0.000	(0)
H2Se	1.561e-18	1.561e-18	-17.807	-17.807	0.000	(0)
Se-2	1.998e-22	8.424e-23	-21.700	-22.074	-0.375	(0)
Se(4)	2.537e-09					
HSeO3-	2.096e-09	1.689e-09	-8.679	-8.772	-0.094	(0)
SeO3-2	4.413e-10	1.861e-10	-9.355	-9.730	-0.375	(0)
H2SeO3	2.142e-14	2.142e-14	-13.669	-13.669	0.000	(0)
FeHSeO3+2	3.204e-21	1.351e-21	-20.494	-20.869	-0.375	(0)
Se(6)	8.670e-23					
SeO4-2	8.658e-23	4.393e-23	-22.063	-22.357	-0.295	(0)
MnSeO4	1.182e-25	1.182e-25	-24.927	-24.927	0.000	(0)
HSeO4-	6.069e-29	4.891e-29	-28.217	-28.311	-0.094	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-48.074	-48.918	-0.844	(0)
U(4)	1.127e-15					
U(OH)5-	1.125e-15	9.066e-16	-14.949	-15.043	-0.094	(0)
U(OH)4	1.543e-18	1.543e-18	-17.812	-17.812	0.000	(0)
U(OH)3+	2.704e-22	2.179e-22	-21.568	-21.662	-0.094	(0)
U(OH)2+2	1.131e-26	4.770e-27	-25.947	-26.321	-0.375	(0)
UOH+3	8.207e-32	1.176e-32	-31.086	-31.930	-0.844	(0)
U(SO4)2	1.043e-33	1.043e-33	-32.982	-32.982	0.000	(0)
USO4+2	1.181e-34	4.981e-35	-33.928	-34.303	-0.375	(0)
U+4	1.117e-37	3.533e-39	-36.952	-38.452	-1.500	(0)
UCl+3	1.680e-39	2.408e-40	-38.775	-39.618	-0.844	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-128.076	-135.669	-7.593	(0)
U(5)	1.117e-15					
UO2+	1.117e-15	9.005e-16	-14.952	-15.046	-0.094	(0)
U(6)	8.459e-09					
Ca2UO2(CO3)3	6.975e-09	7.032e-09	-8.156	-8.153	0.004	(0)
CaUO2(CO3)3-2	1.430e-09	7.254e-10	-8.845	-9.139	-0.295	(0)
UO2(CO3)3-4	4.126e-11	1.305e-12	-10.384	-11.884	-1.500	(0)
UO2(CO3)2-2	8.959e-12	3.778e-12	-11.048	-11.423	-0.375	(0)
MgUO2(CO3)3-2	3.198e-12	1.623e-12	-11.495	-11.790	-0.295	(0)
UO2(OH)2	4.045e-13	4.078e-13	-12.393	-12.390	0.004	(0)
UO2CO3	8.944e-14	8.944e-14	-13.048	-13.048	0.000	(0)
UO2(OH)3-	1.806e-14	1.524e-14	-13.743	-13.817	-0.074	(0)
UO2OH+	1.912e-16	1.541e-16	-15.718	-15.812	-0.094	(0)
UO2SO4	4.020e-17	4.020e-17	-16.396	-16.396	0.000	(0)
UO2+2	1.820e-17	9.235e-18	-16.740	-17.035	-0.295	(0)
UO2(SO4)2-2	3.741e-18	1.578e-18	-17.427	-17.802	-0.375	(0)
(UO2)2CO3(OH)3-	1.192e-18	1.006e-18	-17.924	-17.997	-0.074	(0)
UO2(OH)4-2	1.413e-20	7.171e-21	-19.850	-20.144	-0.295	(0)
UO2Cl+	1.353e-20	1.090e-20	-19.869	-19.962	-0.094	(0)
UO2NO3+	3.364e-23	2.711e-23	-22.473	-22.567	-0.094	(0)

UO2Cl2 6.340e-25 6.392e-25 -24.198 -24.194 0.004 (0)
 (UO2)2(OH)2+2 2.378e-25 1.003e-25 -24.624 -24.999 -0.375 (0)
 (UO2)3(CO3)6-6 4.168e-28 9.289e-31 -27.380 -30.032 -2.652 (0)
 (UO2)2OH+3 2.325e-29 5.052e-30 -28.634 -29.297 -0.663 (0)
 (UO2)3(OH)7- 1.896e-30 1.600e-30 -29.722 -29.796 -0.074 (0)
 (UO2)3(OH)5+ 9.763e-31 7.868e-31 -30.010 -30.104 -0.094 (0)
 (UO2)3(OH)4+2 1.518e-33 7.701e-34 -32.819 -33.113 -0.295 (0)
 (UO2)4(OH)7+ 2.204e-38 1.860e-38 -37.657 -37.730 -0.074 (0)

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

Phase	SI**	log IAP	log K(285 K, 1 atm)
(NH4)2SeO4	-32.90	-32.45	0.45 (NH4)2SeO4
Anhydrite	-0.62	-4.92	-4.31 CaSO4
Aragonite	0.09	-8.12	-8.21 CaCO3
Artinite	-7.18	3.33	10.51 MgCO3:Mg(OH)2:3H2O
Birnessite	-17.43	0.66	18.09 MnO2
Bixbyite	-15.73	-15.44	0.29 Mn2O3
Brucite	-5.77	11.94	17.70 Mg(OH)2
Calcite	0.30	-8.12	-8.42 CaCO3
CaMoO4	-1.94	-9.87	-7.93 CaMoO4
CaSeO3:2H2O	-6.79	-3.83	2.96 CaSeO3:2H2O
CaSeO4:2H2O	-21.93	-24.89	-2.96 CaSeO4:2H2O
CH4(g)	-44.60	-87.58	-42.98 CH4
CO2(g)	-2.37	-20.54	-18.18 CO2
Dolomite(disordered)	-0.53	-16.72	-16.19 CaMg(CO3)2
Dolomite(ordered)	0.07	-16.72	-16.79 CaMg(CO3)2
Epsomite	-3.20	-5.42	-2.21 MgSO4:7H2O
Fe(OH)2	-3.43	10.13	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	7.00	3.96	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-3.59	-2.03	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-13.91	-34.54	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-35.92	-37.83	-1.91 Fe2(SO4)3
Fe3(OH)8	4.13	24.35	20.22 Fe3(OH)8
FeMoO4	-2.16	-12.17	-10.01 FeMoO4
Ferrihydrite	3.36	7.11	3.74 Fe(OH)3
Ferroselite	2.50	-16.45	-18.95 FeSe2
FeSe	-0.52	-11.54	-11.02 FeSe
Goethite	6.16	7.11	0.95 FeOOH
Gummite	-10.36	-2.07	8.28 UO3
Gypsum	-0.31	-4.92	-4.62 CaSO4:2H2O
H-Jarosite	-3.01	-13.37	-10.36 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-9.05	-22.30	-13.25 H2MoO4
H2Se(g)	-16.83	-21.67	-4.84 H2Se
Halite	-7.16	-5.59	1.57 NaCl
Hausmannite	-17.25	46.96	64.20 Mn3O4
Hematite	14.66	14.22	-0.45 Fe2O3
Huntite	-4.78	-33.94	-29.16 CaMg3(CO3)4
Hydromagnesite	-15.38	-22.50	-7.12 Mg5(CO3)4(OH)2:4H2O
K-Jarosite	3.80	-10.01	-13.81 KFe3(SO4)2(OH)6
K2MoO4	-18.86	-15.57	3.29 K2MoO4
K2SeO4	-29.86	-30.59	-0.73 K2SeO4
Lepidocrocite	5.74	7.11	1.37 FeOOH
Lime	-21.73	12.43	34.16 CaO
Maghemite	7.83	14.22	6.39 Fe2O3
Magnesianoferrite	7.19	26.15	18.96 Fe2MgO4
Magnesite	-1.00	-8.61	-7.61 MgCO3
Magnetite	19.38	24.35	4.97 Fe3O4
Manganite	-6.90	18.44	25.34 MnOOH
Melanterite	-4.86	-7.22	-2.36 FeSO4:7H2O
Mg(OH)2(active)	-6.86	11.94	18.79 Mg(OH)2
MgMoO4	-8.51	-10.36	-1.85 MgMoO4
MgSeO3:6H2O	-7.33	-4.32	3.02 MgSeO3:6H2O
MgSeO4:6H2O	-24.18	-25.38	-1.20 MgSeO4:6H2O
Mirabilite	-5.82	-7.54	-1.71 Na2SO4:10H2O

Mn2(SO4)3 -63.01 -67.49 -4.48 Mn2(SO4)3
MnCl2:4H2O -13.73 -10.93 2.80 MnCl2:4H2O
MnSe -15.85 -11.61 4.24 MnSe
MnSeO3 -7.32 -6.19 1.13 MnSeO3
MnSeO3:2H2O -7.11 -6.19 0.92 MnSeO3:2H2O
MnSeO4:5H2O -25.20 -27.25 -2.05 MnSeO4:5H2O
MnSO4 -10.36 -7.29 3.07 MnSO4
MoO3 -14.30 -22.30 -8.00 MoO3
Na-Jarosite 1.59 -8.47 -10.06 NaFe3(SO4)2(OH)6
Na2Mo2O7 -17.76 -34.78 -17.02 Na2Mo2O7
Na2MoO4 -14.05 -12.48 1.57 Na2MoO4
Na2MoO4:2H2O -13.71 -12.48 1.22 Na2MoO4:2H2O
Na2SeO3:5H2O -16.74 -6.44 10.30 Na2SeO3:5H2O
Na2SeO4 -28.78 -27.50 1.28 Na2SeO4
Natron -8.92 -10.73 -1.81 Na2CO3:10H2O
Nesquehonite -4.12 -8.61 -4.49 MgCO3:3H2O
Nsutite -16.84 0.66 17.50 MnO2
O2(g) -53.88 33.52 87.40 O2
Periclase -10.79 11.94 22.72 MgO
Portlandite -11.35 12.43 23.77 Ca(OH)2
Pyrochroite -5.86 10.06 15.93 Mn(OH)2
Pyrolusite -16.61 26.82 43.43 MnO2
Rhodochrosite 0.09 -10.48 -10.57 MnCO3
Rutherfordine -8.14 -22.62 -14.48 UO2CO3
Schoepite -8.44 -2.08 6.37 UO2(OH)2:H2O
Semetal(am) 2.28 -4.91 -7.19 Se
Semetal(hex) 2.92 -4.91 -7.83 Se
SeO2 -16.37 -16.25 0.11 SeO2
SeO3 -59.46 -37.32 22.15 SeO3
Siderite -0.29 -10.41 -10.12 FeCO3
Thenardite -7.93 -7.53 0.39 Na2SO4
Thermonatrite -11.44 -10.73 0.72 Na2CO3:H2O
U3O8 -16.82 7.92 24.74 U3O8
U4O9 -17.57 -17.37 0.20 U4O9
UO2(am) -10.29 -8.53 1.76 UO2
UO2(NO3)2 -41.66 -28.88 12.78 UO2(NO3)2
UO2(NO3)2:2H2O -33.92 -28.88 5.04 UO2(NO3)2:2H2O
UO2(NO3)2:3H2O -32.34 -28.88 3.46 UO2(NO3)2:3H2O
UO2(NO3)2:6H2O -30.77 -28.88 1.89 UO2(NO3)2:6H2O
UO2(OH)2(beta) -8.11 -2.07 6.04 UO2(OH)2
UO2SeO4:4H2O -37.14 -39.39 -2.25 UO2SeO4:4H2O
UO3 -10.39 -2.07 8.31 UO3
Uraninite -4.45 -8.53 -4.08 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 5. SAG1-5

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

Elements	Molality	Moles
Alkalinity	3.043e-03	3.043e-03
Ca	1.005e-02	1.005e-02
Cl	1.130e-03	1.130e-03
Fe(2)	3.301e-05	3.301e-05
Fe(3)	1.794e-06	1.794e-06
K	8.175e-05	8.175e-05
Mg	2.601e-03	2.601e-03
Mn	6.675e-05	6.675e-05
Mo	1.170e-07	1.170e-07
N(-3)	1.366e-05	1.366e-05
N(5)	1.431e-06	1.431e-06
Na	3.173e-03	3.173e-03
O(0)	6.888e-06	6.888e-06

S(-2)	8.124e-07	8.124e-07
S(6)	1.272e-02	1.272e-02
Se	2.284e-09	2.284e-09
U	8.250e-09	8.250e-09

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

pH = 7.440
 pe = 1.600
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 3.927e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.256e-03
 Total CO2 (mol/kg) = 3.256e-03
 Temperature (°C) = 12.90
 Electrical balance (eq) = -8.521e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -1.98
 Iterations = 21 (89 overall)
 Total H = 1.110172e+02
 Total O = 5.556751e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	2.2430	0.1273
N(-3)/N(5)	6.1903	0.3513
O(-2)/O(0)	13.5854	0.7710
S(-2)/S(6)	-3.6067	-0.2047

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.288e-07	1.070e-07	-6.890	-6.971	-0.081	(0)	
H+	4.333e-08	3.631e-08	-7.363	-7.440	-0.077	0.00	
H2O	5.551e+01	9.995e-01	1.744	-0.000	0.000	18.03	
C(4)	3.256e-03						
HCO3-	2.850e-03	2.407e-03	-2.545	-2.619	-0.073	(0)	
H2CO3	2.298e-04	2.298e-04	-3.639	-3.639	0.000	(0)	
CaHCO3+	1.274e-04	1.081e-04	-3.895	-3.966	-0.071	(0)	
MgHCO3+	2.578e-05	2.150e-05	-4.589	-4.668	-0.079	(0)	
CaCO3	9.915e-06	9.915e-06	-5.004	-5.004	0.000	(0)	
CO3-2	4.915e-06	2.422e-06	-5.309	-5.616	-0.307	(0)	
NaHCO3	4.439e-06	4.439e-06	-5.353	-5.353	0.000	(0)	
MgCO3	1.535e-06	1.535e-06	-5.814	-5.814	0.000	(0)	
MnHCO3+	1.105e-06	9.298e-07	-5.957	-6.032	-0.075	(0)	
FeHCO3+	2.652e-07	2.250e-07	-6.577	-6.648	-0.071	(0)	
NaCO3-	1.962e-07	1.656e-07	-6.707	-6.781	-0.073	(0)	
Ca2UO2(CO3)3	6.939e-09	7.002e-09	-8.159	-8.155	0.004	(0)	
CaUO2(CO3)3-2	1.264e-09	6.232e-10	-8.898	-9.205	-0.307	(0)	
UO2(CO3)3-4	3.680e-11	9.559e-13	-10.434	-12.020	-1.585	(0)	
UO2(CO3)2-2	7.543e-12	3.028e-12	-11.122	-11.519	-0.396	(0)	
MgUO2(CO3)3-2	2.409e-12	1.188e-12	-11.618	-11.925	-0.307	(0)	
UO2CO3	7.689e-14	7.689e-14	-13.114	-13.114	0.000	(0)	
(UO2)2CO3(OH)3-	7.198e-19	6.031e-19	-18.143	-18.220	-0.077	(0)	
(UO2)3(CO3)6-6	2.676e-28	4.595e-31	-27.572	-30.338	-2.765	(0)	
Ca	1.005e-02						
Ca+2	6.884e-03	3.393e-03	-2.162	-2.469	-0.307	(0)	
CaSO4	3.028e-03	3.028e-03	-2.519	-2.519	0.000	(0)	
CaHCO3+	1.274e-04	1.081e-04	-3.895	-3.966	-0.071	(0)	
CaCO3	9.915e-06	9.915e-06	-5.004	-5.004	0.000	(0)	
CaNO3+	1.750e-08	1.393e-08	-7.757	-7.856	-0.099	(0)	
CaOH+	7.408e-09	6.285e-09	-8.130	-8.202	-0.071	(0)	
Ca2UO2(CO3)3	6.939e-09	7.002e-09	-8.159	-8.155	0.004	(0)	

CaNH3+2 1.784e-09 7.163e-10 -8.749 -9.145 -0.396 (0)
 CaUO2(CO3)3-2 1.264e-09 6.232e-10 -8.898 -9.205 -0.307 (0)
 Ca(NH3)2+2 1.191e-16 4.781e-17 -15.924 -16.320 -0.396 (0)
 Cl 1.130e-03
 Cl- 1.130e-03 9.472e-04 -2.947 -3.024 -0.077 (0)
 MnCl+ 2.937e-08 2.472e-08 -7.532 -7.607 -0.075 (0)
 MnCl2 3.307e-11 3.307e-11 -10.481 -10.481 0.000 (0)
 MnCl3- 1.025e-14 8.628e-15 -13.989 -14.064 -0.075 (0)
 FeCl+2 2.877e-18 1.444e-18 -17.541 -17.841 -0.299 (0)
 UO2Cl+ 1.254e-20 9.980e-21 -19.902 -20.001 -0.099 (0)
 FeCl2+ 1.075e-20 9.044e-21 -19.969 -20.044 -0.075 (0)
 FeCl3 8.566e-25 8.566e-25 -24.067 -24.067 0.000 (0)
 UO2Cl2 5.687e-25 5.739e-25 -24.245 -24.241 0.004 (0)
 UCl+3 0.000e+00 0.000e+00 -40.028 -40.920 -0.892 (0)
 Fe(2) 3.301e-05
 Fe+2 2.373e-05 9.525e-06 -4.625 -5.021 -0.396 (0)
 FeSO4 8.970e-06 8.970e-06 -5.047 -5.047 0.000 (0)
 FeHCO3+ 2.652e-07 2.250e-07 -6.577 -6.648 -0.071 (0)
 FeOH+ 4.819e-08 4.056e-08 -7.317 -7.392 -0.075 (0)
 Fe(HS)2 1.644e-09 1.644e-09 -8.784 -8.784 0.000 (0)
 Fe(OH)2 3.006e-12 3.006e-12 -11.522 -11.522 0.000 (0)
 Fe(OH)3- 2.787e-13 2.346e-13 -12.555 -12.630 -0.075 (0)
 Fe(HS)3- 9.896e-14 7.877e-14 -13.005 -13.104 -0.099 (0)
 Fe(3) 1.794e-06
 Fe(OH)2+ 1.708e-06 1.442e-06 -5.768 -5.841 -0.073 (0)
 Fe(OH)3 7.305e-08 7.305e-08 -7.136 -7.136 0.000 (0)
 Fe(OH)4- 1.312e-08 1.108e-08 -7.882 -7.955 -0.073 (0)
 FeOH+2 1.306e-11 6.553e-12 -10.884 -11.184 -0.299 (0)
 FeSO4+ 2.859e-15 2.407e-15 -14.544 -14.619 -0.075 (0)
 Fe+3 3.671e-16 7.473e-17 -15.435 -16.127 -0.691 (0)
 Fe(SO4)2- 3.138e-16 2.498e-16 -15.503 -15.602 -0.099 (0)
 FeCl+2 2.877e-18 1.444e-18 -17.541 -17.841 -0.299 (0)
 Fe2(OH)2+4 8.531e-20 2.216e-21 -19.069 -20.654 -1.585 (0)
 FeCl2+ 1.075e-20 9.044e-21 -19.969 -20.044 -0.075 (0)
 FeNO3+2 4.144e-21 1.664e-21 -20.383 -20.779 -0.396 (0)
 FeHSeO3+2 4.866e-22 1.953e-22 -21.313 -21.709 -0.396 (0)
 Fe3(OH)4+5 1.217e-23 4.056e-26 -22.915 -25.392 -2.477 (0)
 FeCl3 8.566e-25 8.566e-25 -24.067 -24.067 0.000 (0)
 H(0) 1.323e-21
 H2 6.616e-22 6.676e-22 -21.179 -21.175 0.004 (0)
 K 8.175e-05
 K+ 7.946e-05 6.658e-05 -4.100 -4.177 -0.077 (0)
 KSO4- 2.289e-06 1.933e-06 -5.640 -5.714 -0.073 (0)
 Mg 2.601e-03
 Mg+2 1.896e-03 9.347e-04 -2.722 -3.029 -0.307 (0)
 MgSO4 6.775e-04 6.775e-04 -3.169 -3.169 0.000 (0)
 MgHCO3+ 2.578e-05 2.150e-05 -4.589 -4.668 -0.079 (0)
 MgCO3 1.535e-06 1.535e-06 -5.814 -5.814 0.000 (0)
 MgOH+ 3.808e-08 3.243e-08 -7.419 -7.489 -0.070 (0)
 MgUO2(CO3)3-2 2.409e-12 1.188e-12 -11.618 -11.925 -0.307 (0)
 Mn(2) 6.675e-05
 Mn+2 5.164e-05 2.073e-05 -4.287 -4.683 -0.396 (0)
 MnSO4 1.397e-05 1.397e-05 -4.855 -4.855 0.000 (0)
 MnHCO3+ 1.105e-06 9.298e-07 -5.957 -6.032 -0.075 (0)
 MnCl+ 2.937e-08 2.472e-08 -7.532 -7.607 -0.075 (0)
 MnOH+ 6.617e-09 5.569e-09 -8.179 -8.254 -0.075 (0)
 MnNO3+ 4.887e-11 3.890e-11 -10.311 -10.410 -0.099 (0)
 MnCl2 3.307e-11 3.307e-11 -10.481 -10.481 0.000 (0)
 MnCl3- 1.025e-14 8.628e-15 -13.989 -14.064 -0.075 (0)
 Mn(NO3)2 1.190e-16 1.190e-16 -15.924 -15.924 0.000 (0)
 Mn(OH)3- 8.143e-18 6.854e-18 -17.089 -17.164 -0.075 (0)
 MnSe 1.489e-21 1.489e-21 -20.827 -20.827 0.000 (0)
 Mn(OH)4-2 1.222e-23 6.134e-24 -22.913 -23.212 -0.299 (0)
 MnSeO4 3.501e-24 3.501e-24 -23.456 -23.456 0.000 (0)
 Mn(3) 2.878e-29
 Mn+3 2.878e-29 5.858e-30 -28.541 -29.232 -0.691 (0)

Mn(6) 0.000e+00
MnO4-2 0.000e+00 0.000e+00 -62.156 -62.456 -0.299 (0)
Mn(7) 0.000e+00
MnO4- 0.000e+00 0.000e+00 -70.972 -71.055 -0.083 (0)
Mo 1.170e-07
MoO4-2 1.169e-07 5.763e-08 -6.932 -7.239 -0.307 (0)
HMoO4- 3.718e-11 2.960e-11 -10.430 -10.529 -0.099 (0)
H2MoO4 1.726e-14 1.726e-14 -13.763 -13.763 0.000 (0)
Mo7O24-6 0.000e+00 0.000e+00 -51.947 -55.515 -3.567 (0)
HMo7O24-5 0.000e+00 0.000e+00 -54.165 -56.642 -2.477 (0)
H2Mo7O24-4 0.000e+00 0.000e+00 -57.737 -59.322 -1.585 (0)
H3Mo7O24-3 0.000e+00 0.000e+00 -62.609 -63.501 -0.892 (0)
N(-3) 1.366e-05
NH4+ 1.299e-05 1.068e-05 -4.886 -4.972 -0.085 (0)
NH4SO4- 5.978e-07 5.031e-07 -6.223 -6.298 -0.075 (0)
NH3 6.904e-08 6.904e-08 -7.161 -7.161 0.000 (0)
CaNH3+2 1.784e-09 7.163e-10 -8.749 -9.145 -0.396 (0)
Ca(NH3)2+2 1.191e-16 4.781e-17 -15.924 -16.320 -0.396 (0)
N(5) 1.431e-06
NO3- 1.413e-06 1.184e-06 -5.850 -5.927 -0.077 (0)
CaNO3+ 1.750e-08 1.393e-08 -7.757 -7.856 -0.099 (0)
MnNO3+ 4.887e-11 3.890e-11 -10.311 -10.410 -0.099 (0)
Mn(NO3)2 1.190e-16 1.190e-16 -15.924 -15.924 0.000 (0)
FeNO3+2 4.144e-21 1.664e-21 -20.383 -20.779 -0.396 (0)
UO2NO3+ 3.109e-23 2.475e-23 -22.507 -22.606 -0.099 (0)
Na 3.173e-03
Na+ 3.097e-03 2.595e-03 -2.509 -2.586 -0.077 (0)
NaSO4- 7.134e-05 6.024e-05 -4.147 -4.220 -0.073 (0)
NaHCO3 4.439e-06 4.439e-06 -5.353 -5.353 0.000 (0)
NaCO3- 1.962e-07 1.656e-07 -6.707 -6.781 -0.073 (0)
O(0) 6.888e-06
O2 3.444e-06 3.476e-06 -5.463 -5.459 0.004 (0)
S(-2) 8.124e-07
HS- 5.528e-07 4.400e-07 -6.257 -6.357 -0.099 (0)
H2S 2.435e-07 2.435e-07 -6.613 -6.613 0.000 (0)
S5-2 6.857e-09 2.753e-09 -8.164 -8.560 -0.396 (0)
S6-2 3.971e-09 1.594e-09 -8.401 -8.798 -0.396 (0)
S4-2 1.690e-09 6.784e-10 -8.772 -9.169 -0.396 (0)
Fe(HS)2 1.644e-09 1.644e-09 -8.784 -8.784 0.000 (0)
S3-2 2.514e-10 1.009e-10 -9.600 -9.996 -0.396 (0)
S2-2 2.255e-11 9.054e-12 -10.647 -11.043 -0.396 (0)
Fe(HS)3- 9.896e-14 7.877e-14 -13.005 -13.104 -0.099 (0)
S-2 5.211e-17 2.615e-17 -16.283 -16.583 -0.299 (0)
S(6) 1.272e-02
SO4-2 8.922e-03 4.397e-03 -2.050 -2.357 -0.307 (0)
CaSO4 3.028e-03 3.028e-03 -2.519 -2.519 0.000 (0)
MgSO4 6.775e-04 6.775e-04 -3.169 -3.169 0.000 (0)
NaSO4- 7.134e-05 6.024e-05 -4.147 -4.220 -0.073 (0)
MnSO4 1.397e-05 1.397e-05 -4.855 -4.855 0.000 (0)
FeSO4 8.970e-06 8.970e-06 -5.047 -5.047 0.000 (0)
KSO4- 2.289e-06 1.933e-06 -5.640 -5.714 -0.073 (0)
NH4SO4- 5.978e-07 5.031e-07 -6.223 -6.298 -0.075 (0)
HSO4- 1.279e-08 1.072e-08 -7.893 -7.970 -0.077 (0)
FeSO4+ 2.859e-15 2.407e-15 -14.544 -14.619 -0.075 (0)
Fe(SO4)2- 3.138e-16 2.498e-16 -15.503 -15.602 -0.099 (0)
UO2SO4 4.039e-17 4.039e-17 -16.394 -16.394 0.000 (0)
UO2(SO4)2-2 4.289e-18 1.722e-18 -17.368 -17.764 -0.396 (0)
U(SO4)2 6.271e-35 6.271e-35 -34.203 -34.203 0.000 (0)
USO4+2 6.852e-36 2.751e-36 -35.164 -35.561 -0.396 (0)
Se(-2) 7.966e-19
HSe- 7.949e-19 6.328e-19 -18.100 -18.199 -0.099 (0)
MnSe 1.489e-21 1.489e-21 -20.827 -20.827 0.000 (0)
H2Se 1.686e-22 1.686e-22 -21.773 -21.773 0.000 (0)
Se-2 1.910e-26 7.668e-27 -25.719 -26.115 -0.396 (0)
Se(4) 2.284e-09
HSeO3- 1.904e-09 1.516e-09 -8.720 -8.819 -0.099 (0)

SeO3-2 3.800e-10 1.525e-10 -9.420 -9.817 -0.396 (0)
 H2SeO3 2.112e-14 2.112e-14 -13.675 -13.675 0.000 (0)
 FeHSeO3+2 4.866e-22 1.953e-22 -21.313 -21.709 -0.396 (0)
 Se(6) 1.620e-21
 SeO4-2 1.617e-21 7.969e-22 -20.791 -21.099 -0.307 (0)
 MnSeO4 3.501e-24 3.501e-24 -23.456 -23.456 0.000 (0)
 HSeO4- 1.230e-27 9.794e-28 -26.910 -27.009 -0.099 (0)
 U(3) 0.000e+00
 U+3 0.000e+00 0.000e+00 -50.005 -50.897 -0.892 (0)
 U(4) 3.795e-17
 U(OH)5- 3.789e-17 3.016e-17 -16.421 -16.521 -0.099 (0)
 U(OH)4 5.610e-20 5.610e-20 -19.251 -19.251 0.000 (0)
 U(OH)3+ 1.089e-23 8.665e-24 -22.963 -23.062 -0.099 (0)
 U(OH)2+2 5.149e-28 2.067e-28 -27.288 -27.685 -0.396 (0)
 UOH+3 4.324e-33 5.546e-34 -32.364 -33.256 -0.892 (0)
 U(SO4)2 6.271e-35 6.271e-35 -34.203 -34.203 0.000 (0)
 USO4+2 6.852e-36 2.751e-36 -35.164 -35.561 -0.396 (0)
 U+4 6.934e-39 1.801e-40 -38.159 -39.744 -1.585 (0)
 UCl+3 0.000e+00 0.000e+00 -40.028 -40.920 -0.892 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -135.999 -144.025 -8.027 (0)
 U(5) 2.078e-16
 UO2+ 2.078e-16 1.654e-16 -15.682 -15.781 -0.099 (0)
 U(6) 8.250e-09
 Ca2UO2(CO3)3 6.939e-09 7.002e-09 -8.159 -8.155 0.004 (0)
 CaUO2(CO3)3-2 1.264e-09 6.232e-10 -8.898 -9.205 -0.307 (0)
 UO2(CO3)3-4 3.680e-11 9.559e-13 -10.434 -12.020 -1.585 (0)
 UO2(CO3)2-2 7.543e-12 3.028e-12 -11.122 -11.519 -0.396 (0)
 MgUO2(CO3)3-2 2.409e-12 1.188e-12 -11.618 -11.925 -0.307 (0)
 UO2(OH)2 3.107e-13 3.135e-13 -12.508 -12.504 0.004 (0)
 UO2CO3 7.689e-14 7.689e-14 -13.114 -13.114 0.000 (0)
 UO2(OH)3- 1.275e-14 1.069e-14 -13.894 -13.971 -0.077 (0)
 UO2OH+ 1.655e-16 1.317e-16 -15.781 -15.880 -0.099 (0)
 UO2SO4 4.039e-17 4.039e-17 -16.394 -16.394 0.000 (0)
 UO2+2 1.732e-17 8.536e-18 -16.762 -17.069 -0.307 (0)
 UO2(SO4)2-2 4.289e-18 1.722e-18 -17.368 -17.764 -0.396 (0)
 (UO2)2CO3(OH)3- 7.198e-19 6.031e-19 -18.143 -18.220 -0.077 (0)
 UO2Cl+ 1.254e-20 9.980e-21 -19.902 -20.001 -0.099 (0)
 UO2(OH)4-2 9.301e-21 4.584e-21 -20.031 -20.339 -0.307 (0)
 UO2NO3+ 3.109e-23 2.475e-23 -22.507 -22.606 -0.099 (0)
 UO2Cl2 5.687e-25 5.739e-25 -24.245 -24.241 0.004 (0)
 (UO2)2(OH)2+2 1.797e-25 7.214e-26 -24.745 -25.142 -0.396 (0)
 (UO2)3(CO3)6-6 2.676e-28 4.595e-31 -27.572 -30.338 -2.765 (0)
 (UO2)2OH+3 1.934e-29 3.936e-30 -28.714 -29.405 -0.691 (0)
 (UO2)3(OH)7- 7.911e-31 6.629e-31 -30.102 -30.179 -0.077 (0)
 (UO2)3(OH)5+ 5.082e-31 4.045e-31 -30.294 -30.393 -0.099 (0)
 (UO2)3(OH)4+2 8.534e-34 4.206e-34 -33.069 -33.376 -0.307 (0)
 (UO2)4(OH)7+ 8.501e-39 7.123e-39 -38.071 -38.147 -0.077 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-31.49	-31.04	0.45 (NH4)2SeO4
Anhydrite	-0.52	-4.83	-4.31 CaSO4
Aragonite	0.13	-8.09	-8.21 CaCO3
Artinite	-7.29	3.20	10.49 MgCO3:Mg(OH)2:3H2O
Birnessite	-15.96	2.13	18.09 MnO2
Bixbyite	-14.10	-13.83	0.28 Mn2O3
Brucite	-5.84	11.85	17.69 Mg(OH)2
Calcite	0.34	-8.09	-8.42 CaCO3
CaMoO4	-1.77	-9.71	-7.94 CaMoO4
CaSeO3:2H2O	-6.81	-3.85	2.96 CaSeO3:2H2O
CaSeO4:2H2O	-20.61	-23.57	-2.96 CaSeO4:2H2O
CH4(g)	-49.86	-92.82	-42.95 CH4
CO2(g)	-2.32	-20.50	-18.18 CO2
Dolomite(disordered)	-0.53	-16.73	-16.20 CaMg(CO3)2

Dolomite(ordered) 0.07 -16.73 -16.80 CaMg(CO3)2
 Epsomite -3.18 -5.39 -2.21 MgSO4·7H2O
 Fe(OH)2 -3.71 9.86 13.56 Fe(OH)2
 Fe(OH)2·7Cl.3 6.09 3.05 -3.04 Fe(OH)2·7Cl.3
 Fe2(OH)4SeO3 -5.43 -3.87 1.55 Fe2(OH)4SeO3
 Fe2(SeO3)3·2H2O -15.77 -36.39 -20.63 Fe2(SeO3)3·2H2O
 Fe2(SO4)3 -37.38 -39.32 -1.94 Fe2(SO4)3
 Fe3(OH)8 2.02 22.24 20.22 Fe3(OH)8
 FeMoO4 -2.25 -12.26 -10.01 FeMoO4
 Ferrihydrite 2.46 6.19 3.73 Fe(OH)3
 Ferroselite -4.39 -23.34 -18.95 FeSe2
 FeS(ppt) -1.07 -3.94 -2.87 FeS
 FeSe -4.76 -15.78 -11.02 FeSe
 Goethite 5.25 6.19 0.94 FeOOH
 Greigite 12.09 -32.94 -45.03 Fe3S4
 Gummite -10.46 -2.19 8.27 UO3
 Gypsum -0.21 -4.83 -4.62 CaSO4·2H2O
 H-Jarosite -5.50 -15.89 -10.39 (H3O)Fe3(SO4)2(OH)6
 H2MoO4 -8.88 -22.12 -13.24 H2MoO4
 H2S(g) -5.79 -13.80 -8.01 H2S
 H2Se(g) -20.79 -25.64 -4.85 H2Se
 Halite -7.18 -5.61 1.58 NaCl
 Hausmannite -15.48 48.67 64.15 Mn3O4
 Hematite 12.85 12.39 -0.46 Fe2O3
 Huntite -4.85 -34.02 -29.17 CaMg3(CO3)4
 Hydromagnesite -15.58 -22.73 -7.15 Mg5(CO3)4(OH)2·4H2O
 K-Jarosite 1.20 -12.63 -13.83 KFe3(SO4)2(OH)6
 K2MoO4 -18.88 -15.59 3.29 K2MoO4
 K2SeO4 -28.72 -29.45 -0.73 K2SeO4
 Lepidocrocite 4.82 6.19 1.37 FeOOH
 Lime -21.73 12.41 34.14 CaO
 Mackinawite -0.34 -3.94 -3.60 FeS
 Maghemite 6.00 12.39 6.39 Fe2O3
 Magnesioferrite 5.31 24.24 18.93 Fe2MgO4
 Magnesite -1.04 -8.65 -7.61 MgCO3
 Magnetite 17.30 22.24 4.95 Fe3O4
 Manganite -6.10 19.24 25.34 MnOOH
 Melanterite -5.02 -7.38 -2.36 FeSO4·7H2O
 Mg(OH)2(active) -6.94 11.85 18.79 Mg(OH)2
 MgMoO4 -8.42 -10.27 -1.85 MgMoO4
 MgSeO3·6H2O -7.43 -4.41 3.02 MgSeO3·6H2O
 MgSeO4·6H2O -22.93 -24.13 -1.20 MgSeO4·6H2O
 Mirabilite -5.83 -7.53 -1.70 Na2SO4·10H2O
 Mn2(SO4)3 -61.04 -65.53 -4.50 Mn2(SO4)3
 MnCl2·4H2O -13.53 -10.73 2.80 MnCl2·4H2O
 MnS(grn) -4.01 -3.60 0.41 MnS
 MnS(pnk) -6.94 -3.60 3.34 MnS
 MnSe -19.67 -15.44 4.23 MnSe
 MnSeO3 -7.19 -6.06 1.13 MnSeO3
 MnSeO3·2H2O -6.98 -6.06 0.92 MnSeO3·2H2O
 MnSeO4·5H2O -23.73 -25.78 -2.05 MnSeO4·5H2O
 MnSO4 -10.10 -7.04 3.06 MnSO4
 MoO3 -14.12 -22.12 -8.00 MoO3
 MoS2 5.35 -67.79 -73.14 MoS2
 Na-Jarosite -0.96 -11.04 -10.08 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -17.52 -34.53 -17.01 Na2Mo2O7
 Na2MoO4 -13.98 -12.41 1.56 Na2MoO4
 Na2MoO4·2H2O -13.64 -12.41 1.22 Na2MoO4·2H2O
 Na2SeO3·5H2O -16.85 -6.55 10.30 Na2SeO3·5H2O
 Na2SeO4 -27.55 -26.27 1.28 Na2SeO4
 Natron -8.99 -10.79 -1.80 Na2CO3·10H2O
 Nesquehonite -4.16 -8.65 -4.49 MgCO3·3H2O
 Nsutite -15.38 2.13 17.50 MnO2
 O2(g) -51.17 36.16 87.33 O2
 Periclase -10.85 11.85 22.70 MgO
 Portlandite -11.35 12.41 23.76 Ca(OH)2

Pyrite 19.22 0.35 -18.88 FeS2
 Pyrochroite -5.72 10.20 15.91 Mn(OH)2
 Pyrolusite -15.12 28.28 43.40 MnO2
 Rhodochrosite 0.27 -10.30 -10.57 MnCO3
 Rutherfordine -8.21 -22.68 -14.48 UO2CO3
 Schoepite -8.55 -2.19 6.36 UO2(OH)2:H2O
 Semetal(am) -0.37 -7.56 -7.19 Se
 Semetal(hex) 0.27 -7.56 -7.83 Se
 SeO2 -16.37 -16.26 0.11 SeO2
 SeO3 -58.11 -35.98 22.13 SeO3
 Siderite -0.52 -10.64 -10.12 FeCO3
 Sulfur 6.31 4.28 -2.02 S
 Thenardite -7.92 -7.53 0.39 Na2SO4
 Thermonatrite -11.50 -10.79 0.71 Na2CO3:H2O
 U3O8 -18.48 6.20 24.68 U3O8
 U4O9 -22.00 -21.86 0.14 U4O9
 UO2(am) -11.73 -9.98 1.75 UO2
 UO2(NO3)2 -41.69 -28.92 12.77 UO2(NO3)2
 UO2(NO3)2:2H2O -33.96 -28.92 5.04 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -32.38 -28.92 3.46 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -30.82 -28.92 1.89 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -8.22 -2.19 6.03 UO2(OH)2
 UO2SeO4:4H2O -35.92 -38.17 -2.25 UO2SeO4:4H2O
 UO3 -10.49 -2.19 8.30 UO3
 Uraninite -5.89 -9.98 -4.09 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 6. SAG2-1

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

Elements	Molality	Moles
Alkalinity	5.221e-03	5.221e-03
Ca	4.396e-03	4.396e-03
Cl	1.525e-03	1.525e-03
Fe(2)	2.868e-06	2.868e-06
Fe(3)	1.075e-06	1.075e-06
K	1.050e-04	1.050e-04
Mg	1.895e-03	1.895e-03
Mn	8.382e-07	8.382e-07
Mo	2.202e-08	2.202e-08
N(-3)	3.573e-06	3.573e-06
N(5)	1.651e-04	1.651e-04
Na	2.843e-03	2.843e-03
O(0)	1.746e-04	1.746e-04
S(6)	4.251e-03	4.251e-03
Se	7.771e-08	7.771e-08
U	2.965e-08	2.965e-08

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

pH = 7.210
 pe = 4.900
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.150e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 5.916e-03
 Total CO2 (mol/kg) = 5.916e-03
 Temperature (°C) = 13.10
 Electrical balance (eq) = 1.279e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.48
 Iterations = 20 (109 overall)
 Total H = 1.110203e+02

Total O = 5.554226e+01

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

Redox couple	pe Eh (volts)	
Fe(2)/Fe(3)	3.4025	0.1932
N(-3)/N(5)	6.7942	0.3859
O(-2)/O(0)	14.1505	0.8037

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	7.400e-08	6.403e-08	-7.131	-7.194	-0.063	(0)	
H+	7.092e-08	6.166e-08	-7.149	-7.210	-0.061	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	
C(4)	5.916e-03						
HCO3-	5.010e-03	4.381e-03	-2.300	-2.358	-0.058	(0)	
H2CO3	7.085e-04	7.085e-04	-3.150	-3.150	0.000	(0)	
CaHCO3+	1.334e-04	1.170e-04	-3.875	-3.932	-0.057	(0)	
MgHCO3+	4.354e-05	3.778e-05	-4.361	-4.423	-0.062	(0)	
NaHCO3	7.574e-06	7.574e-06	-5.121	-5.121	0.000	(0)	
CaCO3	6.337e-06	6.337e-06	-5.198	-5.198	0.000	(0)	
CO3-2	4.563e-06	2.608e-06	-5.341	-5.584	-0.243	(0)	
MgCO3	1.599e-06	1.599e-06	-5.796	-5.796	0.000	(0)	
NaCO3-	1.908e-07	1.668e-07	-6.720	-6.778	-0.058	(0)	
FeHCO3+	5.858e-08	5.137e-08	-7.232	-7.289	-0.057	(0)	
MnHCO3+	3.352e-08	2.925e-08	-7.475	-7.534	-0.059	(0)	
Ca2UO2(CO3)3	2.328e-08	2.339e-08	-7.633	-7.631	0.002	(0)	
CaUO2(CO3)3-2	6.165e-09	3.523e-09	-8.210	-8.453	-0.243	(0)	
UO2(CO3)3-4	1.348e-10	9.039e-12	-9.870	-11.044	-1.174	(0)	
UO2(CO3)2-2	5.314e-11	2.704e-11	-10.275	-10.568	-0.293	(0)	
MgUO2(CO3)3-2	1.917e-11	1.096e-11	-10.717	-10.960	-0.243	(0)	
UO2CO3	6.355e-13	6.355e-13	-12.197	-12.197	0.000	(0)	
(UO2)2CO3(OH)3-	8.932e-18	7.766e-18	-17.049	-17.110	-0.061	(0)	
(UO2)3(CO3)6-6	4.834e-26	3.144e-28	-25.316	-27.503	-2.187	(0)	
Ca	4.396e-03						
Ca+2	3.508e-03	2.005e-03	-2.455	-2.698	-0.243	(0)	
CaSO4	7.466e-04	7.466e-04	-3.127	-3.127	0.000	(0)	
CaHCO3+	1.334e-04	1.170e-04	-3.875	-3.932	-0.057	(0)	
CaCO3	6.337e-06	6.337e-06	-5.198	-5.198	0.000	(0)	
CaNO3+	1.171e-06	9.893e-07	-5.931	-6.005	-0.073	(0)	
Ca2UO2(CO3)3	2.328e-08	2.339e-08	-7.633	-7.631	0.002	(0)	
CaUO2(CO3)3-2	6.165e-09	3.523e-09	-8.210	-8.453	-0.243	(0)	
CaOH+	2.541e-09	2.229e-09	-8.595	-8.652	-0.057	(0)	
CaNH3+2	1.378e-10	7.014e-11	-9.861	-10.154	-0.293	(0)	
Ca(NH3)2+2	1.525e-18	7.758e-19	-17.817	-18.110	-0.293	(0)	
Cl	1.525e-03						
Cl-	1.525e-03	1.326e-03	-2.817	-2.878	-0.061	(0)	
MnCl+	6.843e-10	5.971e-10	-9.165	-9.224	-0.059	(0)	
MnCl2	1.118e-12	1.118e-12	-11.952	-11.952	0.000	(0)	
MnCl3-	4.679e-16	4.083e-16	-15.330	-15.389	-0.059	(0)	
FeCl+2	6.406e-18	3.714e-18	-17.193	-17.430	-0.237	(0)	
UO2Cl+	1.274e-19	1.076e-19	-18.895	-18.968	-0.073	(0)	
FeCl2+	3.707e-20	3.235e-20	-19.431	-19.490	-0.059	(0)	
UO2Cl2	8.578e-24	8.621e-24	-23.067	-23.064	0.002	(0)	
FeCl3	4.288e-24	4.288e-24	-23.368	-23.368	0.000	(0)	
UCl+3	0.000e+00	0.000e+00	-44.930	-45.590	-0.660	(0)	
Fe(2)	2.868e-06						
Fe+2	2.338e-06	1.190e-06	-5.631	-5.925	-0.293	(0)	
FeSO4	4.676e-07	4.676e-07	-6.330	-6.330	0.000	(0)	
FeHCO3+	5.858e-08	5.137e-08	-7.232	-7.289	-0.057	(0)	
FeOH+	3.476e-09	3.033e-09	-8.459	-8.518	-0.059	(0)	
Fe(OH)2	1.349e-13	1.349e-13	-12.870	-12.870	0.000	(0)	

Fe(OH)3-	7.119e-15	6.212e-15	-14.148	-14.207	-0.059	(0)
Fe(3)	1.075e-06					
Fe(OH)2+	1.045e-06	9.134e-07	-5.981	-6.039	-0.058	(0)
Fe(OH)3	2.809e-08	2.809e-08	-7.551	-7.551	0.000	(0)
Fe(OH)4-	2.784e-09	2.434e-09	-8.555	-8.614	-0.058	(0)
FeOH+2	1.230e-11	7.134e-12	-10.910	-11.147	-0.237	(0)
FeSO4+	2.112e-15	1.843e-15	-14.675	-14.734	-0.059	(0)
Fe+3	4.805e-16	1.364e-16	-15.318	-15.865	-0.547	(0)
Fe(SO4)2-	9.414e-17	7.951e-17	-16.026	-16.100	-0.073	(0)
FeCl+2	6.406e-18	3.714e-18	-17.193	-17.430	-0.237	(0)
FeNO3+2	7.108e-19	3.617e-19	-18.148	-18.442	-0.293	(0)
Fe2(OH)2+4	3.887e-20	2.606e-21	-19.410	-20.584	-1.174	(0)
FeCl2+	3.707e-20	3.235e-20	-19.431	-19.490	-0.059	(0)
FeHSeO3+2	2.784e-20	1.416e-20	-19.555	-19.849	-0.293	(0)
FeCl3	4.288e-24	4.288e-24	-23.368	-23.368	0.000	(0)
Fe3(OH)4+5	2.065e-24	3.028e-26	-23.685	-25.519	-1.834	(0)
H(0)	9.605e-28					
H2	4.802e-28	4.826e-28	-27.319	-27.316	0.002	(0)
K	1.050e-04					
K+	1.037e-04	9.018e-05	-3.984	-4.045	-0.061	(0)
KSO4-	1.248e-06	1.091e-06	-5.904	-5.962	-0.058	(0)
Mg	1.895e-03					
Mg+2	1.577e-03	9.012e-04	-2.802	-3.045	-0.243	(0)
MgSO4	2.724e-04	2.724e-04	-3.565	-3.565	0.000	(0)
MgHCO3+	4.354e-05	3.778e-05	-4.361	-4.423	-0.062	(0)
MgCO3	1.599e-06	1.599e-06	-5.796	-5.796	0.000	(0)
MgOH+	2.137e-08	1.879e-08	-7.670	-7.726	-0.056	(0)
MgUO2(CO3)3-2	1.917e-11	1.096e-11	-10.717	-10.960	-0.243	(0)
Mn(2)	8.382e-07					
Mn+2	7.031e-07	3.578e-07	-6.153	-6.446	-0.293	(0)
MnSO4	1.007e-07	1.007e-07	-6.997	-6.997	0.000	(0)
MnHCO3+	3.352e-08	2.925e-08	-7.475	-7.534	-0.059	(0)
MnCl+	6.843e-10	5.971e-10	-9.165	-9.224	-0.059	(0)
MnNO3+	9.569e-11	8.082e-11	-10.019	-10.093	-0.073	(0)
MnOH+	6.595e-11	5.755e-11	-10.181	-10.240	-0.059	(0)
MnCl2	1.118e-12	1.118e-12	-11.952	-11.952	0.000	(0)
Mn(NO3)2	2.975e-14	2.975e-14	-13.527	-13.527	0.000	(0)
MnCl3-	4.679e-16	4.083e-16	-15.330	-15.389	-0.059	(0)
MnSeO4	2.063e-18	2.063e-18	-17.685	-17.685	0.000	(0)
Mn(OH)3-	2.769e-20	2.416e-20	-19.558	-19.617	-0.059	(0)
Mn(OH)4-2	2.197e-26	1.274e-26	-25.658	-25.895	-0.237	(0)
MnSe	2.267e-40	2.267e-40	-39.645	-39.645	0.000	(0)
Mn(3)	7.332e-28					
Mn+3	7.332e-28	2.082e-28	-27.135	-27.681	-0.547	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-52.531	-52.768	-0.237	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-57.988	-58.052	-0.064	(0)
Mo	2.202e-08					
MoO4-2	2.200e-08	1.257e-08	-7.658	-7.901	-0.243	(0)
HMoO4-	1.306e-11	1.103e-11	-10.884	-10.957	-0.073	(0)
H2MoO4	1.078e-14	1.078e-14	-13.968	-13.968	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-55.692	-58.333	-2.641	(0)
HMo7O24-5	0.000e+00	0.000e+00	-57.395	-59.229	-1.834	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-60.505	-61.678	-1.174	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-64.967	-65.628	-0.660	(0)
N(-3)	3.573e-06					
NH4+	3.494e-06	3.005e-06	-5.457	-5.522	-0.066	(0)
NH4SO4-	6.755e-08	5.895e-08	-7.170	-7.230	-0.059	(0)
NH3	1.162e-08	1.162e-08	-7.935	-7.935	0.000	(0)
CaNH3+2	1.378e-10	7.014e-11	-9.861	-10.154	-0.293	(0)
Ca(NH3)2+2	1.525e-18	7.758e-19	-17.817	-18.110	-0.293	(0)
N(5)	1.651e-04					
NO3-	1.639e-04	1.425e-04	-3.785	-3.846	-0.061	(0)
CaNO3+	1.171e-06	9.893e-07	-5.931	-6.005	-0.073	(0)
MnNO3+	9.569e-11	8.082e-11	-10.019	-10.093	-0.073	(0)

Mn(NO3)2	2.975e-14	2.975e-14	-13.527	-13.527	0.000	(0)
FeNO3+2	7.108e-19	3.617e-19	-18.148	-18.442	-0.293	(0)
UO2NO3+	2.695e-20	2.276e-20	-19.569	-19.643	-0.073	(0)
Na	2.843e-03					
Na+	2.809e-03	2.442e-03	-2.552	-2.612	-0.061	(0)
NaSO4-	2.700e-05	2.361e-05	-4.569	-4.627	-0.058	(0)
NaHCO3	7.574e-06	7.574e-06	-5.121	-5.121	0.000	(0)
NaCO3-	1.908e-07	1.668e-07	-6.720	-6.778	-0.058	(0)
O(0)	1.746e-04					
O2	8.728e-05	8.771e-05	-4.059	-4.057	0.002	(0)
S(6)	4.251e-03					
SO4-2	3.204e-03	1.831e-03	-2.494	-2.737	-0.243	(0)
CaSO4	7.466e-04	7.466e-04	-3.127	-3.127	0.000	(0)
MgSO4	2.724e-04	2.724e-04	-3.565	-3.565	0.000	(0)
NaSO4-	2.700e-05	2.361e-05	-4.569	-4.627	-0.058	(0)
KSO4-	1.248e-06	1.091e-06	-5.904	-5.962	-0.058	(0)
FeSO4	4.676e-07	4.676e-07	-6.330	-6.330	0.000	(0)
MnSO4	1.007e-07	1.007e-07	-6.997	-6.997	0.000	(0)
NH4SO4-	6.755e-08	5.895e-08	-7.170	-7.230	-0.059	(0)
HSO4-	8.765e-09	7.628e-09	-8.057	-8.118	-0.060	(0)
FeSO4+	2.112e-15	1.843e-15	-14.675	-14.734	-0.059	(0)
UO2SO4	1.297e-16	1.297e-16	-15.887	-15.887	0.000	(0)
Fe(SO4)2-	9.414e-17	7.951e-17	-16.026	-16.100	-0.073	(0)
UO2(SO4)2-2	4.549e-18	2.315e-18	-17.342	-17.635	-0.293	(0)
U(SO4)2	1.685e-40	1.685e-40	-39.773	-39.773	0.000	(0)
USO4+2	0.000e+00	0.000e+00	-40.460	-40.754	-0.293	(0)
Se(-2)	1.123e-35					
HSe-	1.122e-35	9.479e-36	-34.950	-35.023	-0.073	(0)
H2Se	4.293e-39	4.293e-39	-38.367	-38.367	0.000	(0)
MnSe	2.267e-40	2.267e-40	-39.645	-39.645	0.000	(0)
Se-2	0.000e+00	0.000e+00	-42.870	-43.164	-0.293	(0)
Se(4)	7.771e-08					
HSeO3-	7.074e-08	5.975e-08	-7.150	-7.224	-0.073	(0)
SeO3-2	6.969e-09	3.546e-09	-8.157	-8.450	-0.293	(0)
H2SeO3	1.416e-12	1.416e-12	-11.849	-11.849	0.000	(0)
FeHSeO3+2	2.784e-20	1.416e-20	-19.555	-19.849	-0.293	(0)
Se(6)	4.741e-14					
SeO4-2	4.741e-14	2.709e-14	-13.324	-13.567	-0.243	(0)
MnSeO4	2.063e-18	2.063e-18	-17.685	-17.685	0.000	(0)
HSeO4-	6.741e-20	5.693e-20	-19.171	-19.245	-0.073	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-58.338	-58.998	-0.660	(0)
U(4)	4.030e-23					
U(OH)5-	4.019e-23	3.394e-23	-22.396	-22.469	-0.073	(0)
U(OH)4	1.068e-25	1.068e-25	-24.971	-24.971	0.000	(0)
U(OH)3+	3.308e-29	2.794e-29	-28.480	-28.554	-0.073	(0)
U(OH)2+2	2.211e-33	1.125e-33	-32.655	-32.949	-0.293	(0)
UOH+3	2.326e-38	5.086e-39	-37.633	-38.294	-0.660	(0)
U(SO4)2	1.685e-40	1.685e-40	-39.773	-39.773	0.000	(0)
USO4+2	0.000e+00	0.000e+00	-40.460	-40.754	-0.293	(0)
U+4	0.000e+00	0.000e+00	-43.385	-44.558	-1.174	(0)
UCl+3	0.000e+00	0.000e+00	-44.930	-45.590	-0.660	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-170.415	-176.357	-5.942	(0)
U(5)	7.496e-19					
UO2+	7.496e-19	6.331e-19	-18.125	-18.199	-0.073	(0)
U(6)	2.965e-08					
Ca2UO2(CO3)3	2.328e-08	2.339e-08	-7.633	-7.631	0.002	(0)
CaUO2(CO3)3-2	6.165e-09	3.523e-09	-8.210	-8.453	-0.243	(0)
UO2(CO3)3-4	1.348e-10	9.039e-12	-9.870	-11.044	-1.174	(0)
UO2(CO3)2-2	5.314e-11	2.704e-11	-10.275	-10.568	-0.293	(0)
MgUO2(CO3)3-2	1.917e-11	1.096e-11	-10.717	-10.960	-0.243	(0)
UO2(OH)2	8.297e-13	8.338e-13	-12.081	-12.079	0.002	(0)
UO2CO3	6.355e-13	6.355e-13	-12.197	-12.197	0.000	(0)
UO2(OH)3-	1.925e-14	1.674e-14	-13.716	-13.776	-0.061	(0)
UO2OH+	7.145e-16	6.034e-16	-15.146	-15.219	-0.073	(0)
UO2SO4	1.297e-16	1.297e-16	-15.887	-15.887	0.000	(0)

UO2+2 1.145e-16 6.546e-17 -15.941 -16.184 -0.243 (0)
 (UO2)2CO3(OH)3- 8.932e-18 7.766e-18 -17.049 -17.110 -0.061 (0)
 UO2(SO4)2-2 4.549e-18 2.315e-18 -17.342 -17.635 -0.293 (0)
 UO2Cl+ 1.274e-19 1.076e-19 -18.895 -18.968 -0.073 (0)
 UO2NO3+ 2.695e-20 2.276e-20 -19.569 -19.643 -0.073 (0)
 UO2(OH)4-2 7.401e-21 4.230e-21 -20.131 -20.374 -0.243 (0)
 UO2Cl2 8.578e-24 8.621e-24 -23.067 -23.064 0.002 (0)
 (UO2)2(OH)2+2 2.928e-24 1.490e-24 -23.533 -23.827 -0.293 (0)
 (UO2)3(CO3)6-6 4.834e-26 3.144e-28 -25.316 -27.503 -2.187 (0)
 (UO2)2OH+3 4.801e-28 1.363e-28 -27.319 -27.865 -0.547 (0)
 (UO2)3(OH)5+ 1.580e-29 1.334e-29 -28.801 -28.875 -0.073 (0)
 (UO2)3(OH)7- 8.450e-30 7.347e-30 -29.073 -29.134 -0.061 (0)
 (UO2)3(OH)4+2 3.993e-32 2.282e-32 -31.399 -31.642 -0.243 (0)
 (UO2)4(OH)7+ 6.964e-37 6.055e-37 -36.157 -36.218 -0.061 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-25.06	-24.61	0.45 (NH4)2SeO4
Anhydrite	-1.13	-5.44	-4.31 CaSO4
Aragonite	-0.07	-8.28	-8.21 CaCO3
Artinite	-7.73	2.75	10.48 MgCO3:Mg(OH)2:3H2O
Birnessite	-12.03	6.06	18.09 MnO2
Bixbyite	-12.37	-12.10	0.26 Mn2O3
Brucite	-6.30	11.37	17.67 Mg(OH)2
Calcite	0.14	-8.28	-8.42 CaCO3
CaMoO4	-2.66	-10.60	-7.94 CaMoO4
CaSeO3:2H2O	-5.67	-2.71	2.96 CaSeO3:2H2O
CaSeO4:2H2O	-13.31	-16.27	-2.96 CaSeO4:2H2O
CH4(g)	-73.97	-116.88	-42.92 CH4
CO2(g)	-1.83	-20.00	-18.18 CO2
Dolomite(disordered)	-0.71	-16.91	-16.20 CaMg(CO3)2
Dolomite(ordered)	-0.11	-16.91	-16.80 CaMg(CO3)2
Epsomite	-3.57	-5.78	-2.21 MgSO4:7H2O
Fe(OH)2	-5.07	8.50	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	5.78	2.74	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-4.46	-2.90	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-11.15	-31.77	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-37.97	-39.94	-1.97 Fe2(SO4)3
Fe3(OH)8	-0.20	20.02	20.22 Fe3(OH)8
FeMoO4	-3.81	-13.83	-10.01 FeMoO4
Ferrihydrite	2.04	5.76	3.73 Fe(OH)3
Ferroselite	-32.81	-51.75	-18.94 FeSe2
FeSe	-22.72	-33.74	-11.02 FeSe
Goethite	4.83	5.76	0.93 FeOOH
Gummite	-10.03	-1.76	8.26 UO3
Gypsum	-0.82	-5.44	-4.62 CaSO4:2H2O
H-Jarosite	-6.60	-17.02	-10.42 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-9.09	-22.32	-13.23 H2MoO4
H2Se(g)	-37.38	-42.23	-4.85 H2Se
Halite	-7.07	-5.49	1.58 NaCl
Hausmannite	-15.96	48.14	64.10 Mn3O4
Hematite	12.01	11.53	-0.48 Fe2O3
Huntite	-4.99	-34.17	-29.18 CaMg3(CO3)4
Hydromagnesite	-15.97	-23.14	-7.18 Mg5(CO3)4(OH)2:4H2O
K-Jarosite	-0.01	-13.86	-13.85 KFe3(SO4)2(OH)6
K2MoO4	-19.28	-15.99	3.29 K2MoO4
K2SeO4	-20.93	-21.66	-0.73 K2SeO4
Lepidocrocite	4.39	5.76	1.37 FeOOH
Lime	-22.39	11.72	34.11 CaO
Maghemite	5.14	11.53	6.39 Fe2O3
Magnesioferrite	4.01	22.90	18.89 Fe2MgO4
Magnesite	-1.02	-8.63	-7.61 MgCO3
Magnetite	15.10	20.02	4.92 Fe3O4
Manganite	-5.26	20.08	25.34 MnOOH

Melanterite -6.30 -8.66 -2.36 FeSO4:7H2O
 Mg(OH)2(active) -7.42 11.37 18.79 Mg(OH)2
 MgMoO4 -9.10 -10.95 -1.85 MgMoO4
 MgSeO3:6H2O -6.08 -3.06 3.02 MgSeO3:6H2O
 MgSeO4:6H2O -15.41 -16.61 -1.20 MgSeO4:6H2O
 Mirabilite -6.27 -7.96 -1.69 Na2SO4:10H2O
 Mn2(SO4)3 -59.05 -63.58 -4.52 Mn2(SO4)3
 MnCl2:4H2O -15.00 -12.20 2.79 MnCl2:4H2O
 MnSe -38.47 -34.26 4.21 MnSe
 MnSeO3 -7.59 -6.46 1.13 MnSeO3
 MnSeO3:2H2O -7.38 -6.46 0.92 MnSeO3:2H2O
 MnSeO4:5H2O -17.96 -20.01 -2.05 MnSeO4:5H2O
 MnSO4 -12.24 -9.18 3.06 MnSO4
 MoO3 -14.32 -22.32 -8.00 MoO3
 Na-Jarosite -2.33 -12.42 -10.10 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -18.44 -35.45 -17.01 Na2Mo2O7
 Na2MoO4 -14.69 -13.13 1.56 Na2MoO4
 Na2MoO4:2H2O -14.35 -13.13 1.22 Na2MoO4:2H2O
 Na2SeO3:5H2O -15.54 -5.24 10.30 Na2SeO3:5H2O
 Na2SeO4 -20.07 -18.79 1.28 Na2SeO4
 Natron -9.02 -10.81 -1.79 Na2CO3:10H2O
 Nesquehonite -4.14 -8.63 -4.49 MgCO3:3H2O
 Nsutite -11.45 6.06 17.50 MnO2
 O2(g) -38.81 48.44 87.25 O2
 Periclase -11.31 11.37 22.69 MgO
 Portlandite -12.02 11.72 23.74 Ca(OH)2
 Pyrochroite -7.93 7.97 15.90 Mn(OH)2
 Pyrolusite -11.17 32.19 43.36 MnO2
 Rhodochrosite -1.46 -12.03 -10.57 MnCO3
 Rutherfordine -7.29 -21.77 -14.48 UO2CO3
 Schoepite -8.12 -1.76 6.36 UO2(OH)2:H2O
 Semetal(am) -10.82 -18.01 -7.19 Se
 Semetal(hex) -10.19 -18.01 -7.82 Se
 SeO2 -14.55 -14.43 0.11 SeO2
 SeO3 -50.10 -27.99 22.11 SeO3
 Siderite -1.38 -11.51 -10.12 FeCO3
 Thenardite -8.35 -7.96 0.39 Na2SO4
 Thermonatrite -11.52 -10.81 0.71 Na2CO3:H2O
 U3O8 -23.33 1.28 24.62 U3O8
 U4O9 -38.74 -38.65 0.09 U4O9
 UO2(am) -17.45 -15.72 1.73 UO2
 UO2(NO3)2 -36.63 -23.88 12.75 UO2(NO3)2
 UO2(NO3)2:2H2O -28.91 -23.88 5.04 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -27.33 -23.88 3.46 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -25.77 -23.88 1.89 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -7.79 -1.76 6.02 UO2(OH)2
 UO2SeO4:4H2O -27.50 -29.75 -2.25 UO2SeO4:4H2O
 UO3 -10.05 -1.76 8.29 UO3
 Uraninite -11.62 -15.72 -4.10 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 7. SAG2-2

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

Elements	Molality	Moles
Alkalinity	5.321e-03	5.321e-03
Ca	4.296e-03	4.296e-03
Cl	1.570e-03	1.570e-03
Fe(2)	1.792e-07	1.792e-07
Fe(3)	8.962e-07	8.962e-07
K	1.027e-04	1.027e-04
Mg	1.878e-03	1.878e-03

Mn	9.657e-07	9.657e-07
Mo	2.880e-08	2.880e-08
N(-3)	3.573e-06	3.573e-06
N(5)	1.558e-04	1.558e-04
Na	2.769e-03	2.769e-03
O(0)	1.376e-04	1.376e-04
S(6)	4.272e-03	4.272e-03
Se	7.378e-08	7.378e-08
U	2.956e-08	2.956e-08

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

pH = 7.260
 pe = 5.500
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.140e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 5.957e-03
 Total CO2 (mol/kg) = 5.957e-03
 Temperature (°C) = 12.40
 Electrical balance (eq) = -3.641e-04
 Percent error, 100*(Cat-|An|)/(|Cat+|An|) = -1.38
 Iterations = 22 (131 overall)
 Total H = 1.110203e+02
 Total O = 5.554240e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	4.4458	0.2519
N(-3)/N(5)	6.7723	0.3837
O(-2)/O(0)	14.1285	0.8005

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	7.835e-08	6.783e-08	-7.106	-7.169	-0.063	(0)	
H+	6.318e-08	5.495e-08	-7.199	-7.260	-0.061	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	
C(4)	5.957e-03						
HCO3-	5.111e-03	4.471e-03	-2.292	-2.350	-0.058	(0)	
H2CO3	6.504e-04	6.504e-04	-3.187	-3.187	0.000	(0)	
CaHCO3+	1.303e-04	1.143e-04	-3.885	-3.942	-0.057	(0)	
MgHCO3+	4.384e-05	3.806e-05	-4.358	-4.419	-0.061	(0)	
NaHCO3	7.636e-06	7.636e-06	-5.117	-5.117	0.000	(0)	
CaCO3	6.873e-06	6.873e-06	-5.163	-5.163	0.000	(0)	
CO3-2	5.137e-06	2.941e-06	-5.289	-5.531	-0.242	(0)	
MgCO3	1.765e-06	1.765e-06	-5.753	-5.753	0.000	(0)	
NaCO3-	2.139e-07	1.871e-07	-6.670	-6.728	-0.058	(0)	
MnHCO3+	3.926e-08	3.428e-08	-7.406	-7.465	-0.059	(0)	
Ca2UO2(CO3)3	2.310e-08	2.322e-08	-7.636	-7.634	0.002	(0)	
CaUO2(CO3)3-2	6.248e-09	3.577e-09	-8.204	-8.446	-0.242	(0)	
FeHCO3+	3.682e-09	3.231e-09	-8.434	-8.491	-0.057	(0)	
UO2(CO3)3-4	1.445e-10	9.782e-12	-9.840	-11.010	-1.170	(0)	
UO2(CO3)2-2	4.802e-11	2.449e-11	-10.319	-10.611	-0.292	(0)	
MgUO2(CO3)3-2	1.970e-11	1.128e-11	-10.706	-10.948	-0.242	(0)	
UO2CO3	5.167e-13	5.167e-13	-12.287	-12.287	0.000	(0)	
(UO2)2CO3(OH)3-	7.567e-18	6.583e-18	-17.121	-17.182	-0.061	(0)	
(UO2)3(CO3)6-6	4.067e-26	2.686e-28	-25.391	-27.571	-2.180	(0)	
Ca	4.296e-03						
Ca+2	3.424e-03	1.960e-03	-2.465	-2.708	-0.242	(0)	
CaSO4	7.337e-04	7.337e-04	-3.134	-3.134	0.000	(0)	
CaHCO3+	1.303e-04	1.143e-04	-3.885	-3.942	-0.057	(0)	

CaCO3	6.873e-06	6.873e-06	-5.163	-5.163	0.000	(0)
CaNO3+	1.087e-06	9.183e-07	-5.964	-6.037	-0.073	(0)
Ca2UO2(CO3)3	2.310e-08	2.322e-08	-7.636	-7.634	0.002	(0)
CaUO2(CO3)3-2	6.248e-09	3.577e-09	-8.204	-8.446	-0.242	(0)
CaOH+	2.608e-09	2.289e-09	-8.584	-8.640	-0.057	(0)
CaNH3+2	1.508e-10	7.694e-11	-9.821	-10.114	-0.292	(0)
Ca(NH3)2+2	1.872e-18	9.549e-19	-17.728	-18.020	-0.292	(0)
Cl	1.570e-03					
Cl-	1.570e-03	1.366e-03	-2.804	-2.865	-0.061	(0)
MnCl+	8.125e-10	7.093e-10	-9.090	-9.149	-0.059	(0)
MnCl2	1.368e-12	1.368e-12	-11.864	-11.864	0.000	(0)
MnCl3-	5.895e-16	5.146e-16	-15.230	-15.289	-0.059	(0)
FeCl+2	4.257e-18	2.472e-18	-17.371	-17.607	-0.236	(0)
UO2Cl+	9.341e-20	7.894e-20	-19.030	-19.103	-0.073	(0)
FeCl2+	2.601e-20	2.271e-20	-19.585	-19.644	-0.059	(0)
UO2Cl2	6.590e-24	6.622e-24	-23.181	-23.179	0.002	(0)
FeCl3	3.101e-24	3.101e-24	-23.509	-23.509	0.000	(0)
UCl+3	0.000e+00	0.000e+00	-46.386	-47.044	-0.658	(0)
Fe(2)	1.792e-07					
Fe+2	1.459e-07	7.444e-08	-6.836	-7.128	-0.292	(0)
FeSO4	2.938e-08	2.938e-08	-7.532	-7.532	0.000	(0)
FeHCO3+	3.682e-09	3.231e-09	-8.434	-8.491	-0.057	(0)
FeOH+	2.303e-10	2.010e-10	-9.638	-9.697	-0.059	(0)
Fe(OH)2	9.394e-15	9.394e-15	-14.027	-14.027	0.000	(0)
Fe(OH)3-	5.521e-16	4.820e-16	-15.258	-15.317	-0.059	(0)
Fe(3)	8.962e-07					
Fe(OH)2+	8.697e-07	7.608e-07	-6.061	-6.119	-0.058	(0)
Fe(OH)3	2.359e-08	2.359e-08	-7.627	-7.627	0.000	(0)
Fe(OH)4-	2.918e-09	2.553e-09	-8.535	-8.593	-0.058	(0)
FeOH+2	8.734e-12	5.072e-12	-11.059	-11.295	-0.236	(0)
FeSO4+	1.379e-15	1.203e-15	-14.861	-14.920	-0.059	(0)
Fe+3	3.167e-16	9.027e-17	-15.499	-16.044	-0.545	(0)
Fe(SO4)2-	6.259e-17	5.289e-17	-16.204	-16.277	-0.073	(0)
FeCl+2	4.257e-18	2.472e-18	-17.371	-17.607	-0.236	(0)
FeNO3+2	4.602e-19	2.347e-19	-18.337	-18.629	-0.292	(0)
FeCl2+	2.601e-20	2.271e-20	-19.585	-19.644	-0.059	(0)
Fe2(OH)2+4	1.999e-20	1.353e-21	-19.699	-20.869	-1.170	(0)
FeHSeO3+2	1.684e-20	8.589e-21	-19.774	-20.066	-0.292	(0)
FeCl3	3.101e-24	3.101e-24	-23.509	-23.509	0.000	(0)
Fe3(OH)4+5	8.732e-25	1.299e-26	-24.059	-25.886	-1.827	(0)
H(0)	4.850e-29					
H2	2.425e-29	2.437e-29	-28.615	-28.613	0.002	(0)
K	1.027e-04					
K+	1.014e-04	8.823e-05	-3.994	-4.054	-0.061	(0)
KSO4-	1.231e-06	1.077e-06	-5.910	-5.968	-0.058	(0)
Mg	1.878e-03					
Mg+2	1.561e-03	8.934e-04	-2.807	-3.049	-0.242	(0)
MgSO4	2.719e-04	2.719e-04	-3.566	-3.566	0.000	(0)
MgHCO3+	4.384e-05	3.806e-05	-4.358	-4.419	-0.061	(0)
MgCO3	1.765e-06	1.765e-06	-5.753	-5.753	0.000	(0)
MgOH+	2.216e-08	1.949e-08	-7.655	-7.710	-0.056	(0)
MgUO2(CO3)3-2	1.970e-11	1.128e-11	-10.706	-10.948	-0.242	(0)
Mn(2)	9.657e-07					
Mn+2	8.089e-07	4.126e-07	-6.092	-6.384	-0.292	(0)
MnSO4	1.165e-07	1.165e-07	-6.934	-6.934	0.000	(0)
MnHCO3+	3.926e-08	3.428e-08	-7.406	-7.465	-0.059	(0)
MnCl+	8.125e-10	7.093e-10	-9.090	-9.149	-0.059	(0)
MnNO3+	1.041e-10	8.800e-11	-9.982	-10.056	-0.073	(0)
MnOH+	8.053e-11	7.030e-11	-10.094	-10.153	-0.059	(0)
MnCl2	1.368e-12	1.368e-12	-11.864	-11.864	0.000	(0)
Mn(NO3)2	3.064e-14	3.064e-14	-13.514	-13.514	0.000	(0)
MnCl3-	5.895e-16	5.146e-16	-15.230	-15.289	-0.059	(0)
MnSeO4	4.013e-17	4.013e-17	-16.397	-16.397	0.000	(0)
Mn(OH)3-	4.509e-20	3.936e-20	-19.346	-19.405	-0.059	(0)
Mn(OH)4-2	4.008e-26	2.328e-26	-25.397	-25.633	-0.236	(0)
MnSe	0.000e+00	0.000e+00	-43.459	-43.459	0.000	(0)

Mn(3) 3.001e-27
Mn+3 3.001e-27 8.555e-28 -26.523 -27.068 -0.545 (0)
Mn(6) 0.000e+00
MnO4-2 0.000e+00 0.000e+00 -49.988 -50.224 -0.236 (0)
Mn(7) 0.000e+00
MnO4- 0.000e+00 0.000e+00 -54.895 -54.958 -0.064 (0)
Mo 2.880e-08
MoO4-2 2.878e-08 1.648e-08 -7.541 -7.783 -0.242 (0)
HMoO4- 1.493e-11 1.262e-11 -10.826 -10.899 -0.073 (0)
H2MoO4 1.152e-14 1.152e-14 -13.939 -13.939 0.000 (0)
Mo7O24-6 0.000e+00 0.000e+00 -55.177 -57.809 -2.631 (0)
HMo7O24-5 0.000e+00 0.000e+00 -56.932 -58.759 -1.827 (0)
H2Mo7O24-4 0.000e+00 0.000e+00 -60.091 -61.260 -1.170 (0)
H3Mo7O24-3 0.000e+00 0.000e+00 -64.601 -65.259 -0.658 (0)
N(-3) 3.573e-06
NH4+ 3.492e-06 3.005e-06 -5.457 -5.522 -0.065 (0)
NH4SO4- 6.839e-08 5.970e-08 -7.165 -7.224 -0.059 (0)
NH3 1.236e-08 1.236e-08 -7.908 -7.908 0.000 (0)
CaNH3+2 1.508e-10 7.694e-11 -9.821 -10.114 -0.292 (0)
Ca(NH3)2+2 1.872e-18 9.549e-19 -17.728 -18.020 -0.292 (0)
N(5) 1.558e-04
NO3- 1.547e-04 1.346e-04 -3.810 -3.871 -0.061 (0)
CaNO3+ 1.087e-06 9.183e-07 -5.964 -6.037 -0.073 (0)
MnNO3+ 1.041e-10 8.800e-11 -9.982 -10.056 -0.073 (0)
Mn(NO3)2 3.064e-14 3.064e-14 -13.514 -13.514 0.000 (0)
FeNO3+2 4.602e-19 2.347e-19 -18.337 -18.629 -0.292 (0)
UO2NO3+ 1.864e-20 1.575e-20 -19.729 -19.803 -0.073 (0)
Na 2.769e-03
Na+ 2.735e-03 2.379e-03 -2.563 -2.624 -0.061 (0)
NaSO4- 2.660e-05 2.327e-05 -4.575 -4.633 -0.058 (0)
NaHCO3 7.636e-06 7.636e-06 -5.117 -5.117 0.000 (0)
NaCO3- 2.139e-07 1.871e-07 -6.670 -6.728 -0.058 (0)
O(0) 1.376e-04
O2 6.882e-05 6.916e-05 -4.162 -4.160 0.002 (0)
S(6) 4.272e-03
SO4-2 3.239e-03 1.854e-03 -2.490 -2.732 -0.242 (0)
CaSO4 7.337e-04 7.337e-04 -3.134 -3.134 0.000 (0)
MgSO4 2.719e-04 2.719e-04 -3.566 -3.566 0.000 (0)
NaSO4- 2.660e-05 2.327e-05 -4.575 -4.633 -0.058 (0)
KSO4- 1.231e-06 1.077e-06 -5.910 -5.968 -0.058 (0)
MnSO4 1.165e-07 1.165e-07 -6.934 -6.934 0.000 (0)
NH4SO4- 6.839e-08 5.970e-08 -7.165 -7.224 -0.059 (0)
FeSO4 2.938e-08 2.938e-08 -7.532 -7.532 0.000 (0)
HSO4- 7.731e-09 6.731e-09 -8.112 -8.172 -0.060 (0)
FeSO4+ 1.379e-15 1.203e-15 -14.861 -14.920 -0.059 (0)
UO2SO4 9.315e-17 9.315e-17 -16.031 -16.031 0.000 (0)
Fe(SO4)2- 6.259e-17 5.289e-17 -16.204 -16.277 -0.073 (0)
UO2(SO4)2-2 3.240e-18 1.653e-18 -17.489 -17.782 -0.292 (0)
U(SO4)2 0.000e+00 0.000e+00 -41.253 -41.253 0.000 (0)
USO4+2 0.000e+00 0.000e+00 -41.935 -42.228 -0.292 (0)
Se(-2) 1.328e-39
HSe- 1.328e-39 1.122e-39 -38.877 -38.950 -0.073 (0)
H2Se 0.000e+00 0.000e+00 -42.345 -42.345 0.000 (0)
MnSe 0.000e+00 0.000e+00 -43.459 -43.459 0.000 (0)
Se-2 0.000e+00 0.000e+00 -46.770 -47.062 -0.292 (0)
Se(4) 7.378e-08
HSeO3- 6.648e-08 5.619e-08 -7.177 -7.250 -0.073 (0)
SeO3-2 7.298e-09 3.722e-09 -8.137 -8.429 -0.292 (0)
H2SeO3 1.179e-12 1.179e-12 -11.928 -11.928 0.000 (0)
FeHSeO3+2 1.684e-20 8.589e-21 -19.774 -20.066 -0.292 (0)
Se(6) 8.099e-13
SeO4-2 8.098e-13 4.636e-13 -12.092 -12.334 -0.242 (0)
MnSeO4 4.013e-17 4.013e-17 -16.397 -16.397 0.000 (0)
HSeO4- 1.003e-18 8.479e-19 -17.999 -18.072 -0.073 (0)
U(3) 0.000e+00
U+3 0.000e+00 0.000e+00 -60.462 -61.119 -0.658 (0)

U(4) 2.125e-24
 U(OH)5- 2.120e-24 1.792e-24 -23.674 -23.747 -0.073 (0)
 U(OH)4 5.087e-27 5.087e-27 -26.294 -26.294 0.000 (0)
 U(OH)3+ 1.416e-30 1.197e-30 -29.849 -29.922 -0.073 (0)
 U(OH)2+2 8.601e-35 4.387e-35 -34.065 -34.358 -0.292 (0)
 UOH+3 8.261e-40 1.816e-40 -39.083 -39.741 -0.658 (0)
 U(SO4)2 0.000e+00 0.000e+00 -41.253 -41.253 0.000 (0)
 USO4+2 0.000e+00 0.000e+00 -41.935 -42.228 -0.292 (0)
 U+4 0.000e+00 0.000e+00 -44.865 -46.034 -1.170 (0)
 UCl+3 0.000e+00 0.000e+00 -46.386 -47.044 -0.658 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -178.541 -184.462 -5.921 (0)
 U(5) 1.382e-19
 UO2+ 1.382e-19 1.168e-19 -18.860 -18.933 -0.073 (0)
 U(6) 2.956e-08
 Ca2UO2(CO3)3 2.310e-08 2.322e-08 -7.636 -7.634 0.002 (0)
 CaUO2(CO3)3-2 6.248e-09 3.577e-09 -8.204 -8.446 -0.242 (0)
 UO2(CO3)3-4 1.445e-10 9.782e-12 -9.840 -11.010 -1.170 (0)
 UO2(CO3)2-2 4.802e-11 2.449e-11 -10.319 -10.611 -0.292 (0)
 MgUO2(CO3)3-2 1.970e-11 1.128e-11 -10.706 -10.948 -0.242 (0)
 UO2(OH)2 7.562e-13 7.600e-13 -12.121 -12.119 0.002 (0)
 UO2CO3 5.167e-13 5.167e-13 -12.287 -12.287 0.000 (0)
 UO2(OH)3- 1.968e-14 1.712e-14 -13.706 -13.767 -0.061 (0)
 UO2OH+ 5.521e-16 4.666e-16 -15.258 -15.331 -0.073 (0)
 UO2SO4 9.315e-17 9.315e-17 -16.031 -16.031 0.000 (0)
 UO2+2 8.278e-17 4.739e-17 -16.082 -16.324 -0.242 (0)
 (UO2)2CO3(OH)3- 7.567e-18 6.583e-18 -17.121 -17.182 -0.061 (0)
 UO2(SO4)2-2 3.240e-18 1.653e-18 -17.489 -17.782 -0.292 (0)
 UO2Cl+ 9.341e-20 7.894e-20 -19.030 -19.103 -0.073 (0)
 UO2NO3+ 1.864e-20 1.575e-20 -19.729 -19.803 -0.073 (0)
 UO2(OH)4-2 8.477e-21 4.853e-21 -20.072 -20.314 -0.242 (0)
 UO2Cl2 6.590e-24 6.622e-24 -23.181 -23.179 0.002 (0)
 (UO2)2(OH)2+2 1.846e-24 9.414e-25 -23.734 -24.026 -0.292 (0)
 (UO2)3(CO3)6-6 4.067e-26 2.686e-28 -25.391 -27.571 -2.180 (0)
 (UO2)2OH+3 2.812e-28 8.017e-29 -27.551 -28.096 -0.545 (0)
 (UO2)3(OH)5+ 9.531e-30 8.055e-30 -29.021 -29.094 -0.073 (0)
 (UO2)3(OH)7- 7.174e-30 6.240e-30 -29.144 -29.205 -0.061 (0)
 (UO2)3(OH)4+2 2.397e-32 1.372e-32 -31.620 -31.863 -0.242 (0)
 (UO2)4(OH)7+ 4.280e-37 3.723e-37 -36.369 -36.429 -0.061 (0)

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

Phase	SI**	log IAP	log K(285 K, 1 atm)
(NH4)2SeO4	-23.83	-23.38	0.45 (NH4)2SeO4
Anhydrite	-1.14	-5.44	-4.30 CaSO4
Aragonite	-0.03	-8.24	-8.21 CaCO3
Artinite	-7.64	2.89	10.53 MgCO3:Mg(OH)2:3H2O
Birnessite	-10.62	7.47	18.09 MnO2
Bixbyite	-10.89	-10.58	0.32 Mn2O3
Brucite	-6.25	11.47	17.73 Mg(OH)2
Calcite	0.18	-8.24	-8.42 CaCO3
CaMoO4	-2.56	-10.49	-7.93 CaMoO4
CaSeO3:2H2O	-5.66	-2.70	2.96 CaSeO3:2H2O
CaSeO4:2H2O	-12.09	-15.04	-2.96 CaSeO4:2H2O
CH4(g)	-79.10	-122.13	-43.03 CH4
CO2(g)	-1.87	-20.05	-18.18 CO2
Dolomite(disordered)	-0.64	-16.82	-16.18 CaMg(CO3)2
Dolomite(ordered)	-0.03	-16.82	-16.78 CaMg(CO3)2
Epsomite	-3.57	-5.78	-2.22 MgSO4:7H2O
Fe(OH)2	-6.17	7.39	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	5.74	2.70	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-4.59	-3.04	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-11.43	-32.06	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-38.42	-40.28	-1.86 Fe2(SO4)3
Fe3(OH)8	-1.36	18.86	20.22 Fe3(OH)8
FeMoO4	-4.91	-14.91	-10.01 FeMoO4

Ferrihydrite	1.98	5.74	3.76	Fe(OH) ₃
Ferroselite	-40.55	-59.51	-18.96	FeSe ₂
FeSe	-27.80	-38.82	-11.02	FeSe
Goethite	4.78	5.74	0.96	FeOOH
Gummite	-10.10	-1.80	8.30	UO ₃
Gypsum	-0.82	-5.44	-4.62	CaSO ₄ :2H ₂ O
H-Jarosite	-6.98	-17.30	-10.32	(H ₃ O)Fe ₃ (SO ₄) ₂ (OH) ₆
H ₂ MoO ₄	-9.05	-22.30	-13.26	H ₂ MoO ₄
H ₂ Se(g)	-41.37	-46.21	-4.84	H ₂ Se
Halite	-7.06	-5.49	1.57	NaCl
Hausmannite	-14.36	49.93	64.28	Mn ₃ O ₄
Hematite	11.89	11.47	-0.42	Fe ₂ O ₃
Huntite	-4.85	-33.98	-29.13	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-15.77	-22.85	-7.08	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
K-Jarosite	-0.30	-14.09	-13.79	KFe ₃ (SO ₄) ₂ (OH) ₆
K ₂ MoO ₄	-19.18	-15.89	3.29	K ₂ MoO ₄
K ₂ SeO ₄	-19.71	-20.44	-0.73	K ₂ SeO ₄
Lepidocrocite	4.36	5.74	1.37	FeOOH
Lime	-22.39	11.81	34.20	CaO
Maghemite	5.08	11.47	6.39	Fe ₂ O ₃
Magnesioferrite	3.93	22.94	19.02	Fe ₂ MgO ₄
Magnesite	-0.97	-8.58	-7.61	MgCO ₃
Magnetite	13.85	18.86	5.01	Fe ₃ O ₄
Manganite	-4.44	20.90	25.34	MnOOH
Melanterite	-7.49	-9.86	-2.37	FeSO ₄ :7H ₂ O
Mg(OH) ₂ (active)	-7.32	11.47	18.79	Mg(OH) ₂
MgMoO ₄	-8.98	-10.83	-1.85	MgMoO ₄
MgSeO ₃ :6H ₂ O	-6.06	-3.04	3.01	MgSeO ₃ :6H ₂ O
MgSeO ₄ :6H ₂ O	-14.18	-15.38	-1.20	MgSeO ₄ :6H ₂ O
Mirabilite	-6.25	-7.98	-1.73	Na ₂ SO ₄ :10H ₂ O
Mn ₂ (SO ₄) ₃	-57.88	-62.33	-4.45	Mn ₂ (SO ₄) ₃
MnCl ₂ :4H ₂ O	-14.91	-12.11	2.80	MnCl ₂ :4H ₂ O
MnSe	-42.33	-38.07	4.26	MnSe
MnSeO ₃	-7.50	-6.37	1.13	MnSeO ₃
MnSeO ₃ :2H ₂ O	-7.29	-6.38	0.92	MnSeO ₃ :2H ₂ O
MnSeO ₄ :5H ₂ O	-16.67	-18.72	-2.05	MnSeO ₄ :5H ₂ O
MnSO ₄	-12.20	-9.12	3.08	MnSO ₄
MoO ₃	-14.30	-22.30	-8.00	MoO ₃
Na-Jarosite	-2.63	-12.66	-10.03	NaFe ₃ (SO ₄) ₂ (OH) ₆
Na ₂ Mo ₂ O ₇	-18.30	-35.33	-17.03	Na ₂ Mo ₂ O ₇
Na ₂ MoO ₄	-14.60	-13.03	1.57	Na ₂ MoO ₄
Na ₂ MoO ₄ :2H ₂ O	-14.25	-13.03	1.22	Na ₂ MoO ₄ :2H ₂ O
Na ₂ SeO ₃ :5H ₂ O	-15.54	-5.24	10.30	Na ₂ SeO ₃ :5H ₂ O
Na ₂ SeO ₄	-18.86	-17.58	1.28	Na ₂ SeO ₄
Natron	-8.96	-10.78	-1.82	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-4.10	-8.58	-4.48	MgCO ₃ :3H ₂ O
Nsutite	-10.03	7.47	17.50	MnO ₂
O ₂ (g)	-36.47	51.04	87.51	O ₂
Periclase	-11.28	11.47	22.75	MgO
Portlandite	-11.99	11.81	23.80	Ca(OH) ₂
Pyrochroite	-7.81	8.14	15.94	Mn(OH) ₂
Pyrolusite	-9.83	33.66	43.48	MnO ₂
Rhodochrosite	-1.35	-11.92	-10.57	MnCO ₃
Rutherfordine	-7.38	-21.86	-14.48	UO ₂ CO ₃
Schoepite	-8.18	-1.80	6.38	UO ₂ (OH) ₂ :H ₂ O
Semetal(am)	-13.50	-20.69	-7.19	Se
Semetal(hex)	-12.86	-20.69	-7.83	Se
SeO ₂	-14.62	-14.51	0.11	SeO ₂
SeO ₃	-49.03	-26.85	22.18	SeO ₃
Siderite	-2.54	-12.66	-10.12	FeCO ₃
Thenardite	-8.37	-7.98	0.39	Na ₂ SO ₄
Thermonatrite	-11.50	-10.78	0.72	Na ₂ CO ₃ :H ₂ O
U ₃ O ₈	-24.78	0.06	24.84	U ₃ O ₈
U ₄ O ₉	-42.74	-42.46	0.28	U ₄ O ₉
UO ₂ (am)	-18.78	-16.99	1.78	UO ₂
UO ₂ (NO ₃) ₂	-36.86	-24.07	12.79	UO ₂ (NO ₃) ₂

UO2(NO3)2:2H2O -29.11 -24.07 5.05 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -27.53 -24.07 3.46 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -25.95 -24.07 1.89 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -7.85 -1.80 6.05 UO2(OH)2
 UO2SeO4:4H2O -26.41 -28.66 -2.25 UO2SeO4:4H2O
 UO3 -10.13 -1.80 8.33 UO3
 Uraninite -12.93 -16.99 -4.07 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 8. SAG2-3

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

Elements	Molality	Moles
Alkalinity	5.501e-03	5.501e-03
Ca	4.396e-03	4.396e-03
Cl	1.601e-03	1.601e-03
Fe(2)	1.792e-05	1.792e-05
Fe(3)	3.585e-06	3.585e-06
K	1.060e-04	1.060e-04
Mg	1.915e-03	1.915e-03
Mn	1.525e-05	1.525e-05
Mo	1.116e-07	1.116e-07
N(-3)	7.075e-06	7.075e-06
N(5)	1.787e-06	1.787e-06
Na	2.952e-03	2.952e-03
O(0)	5.005e-06	5.005e-06
S(6)	4.283e-03	4.283e-03
Se	4.615e-08	4.615e-08
U	3.322e-08	3.322e-08

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

pH = 7.250
 pe = 2.600
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.179e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 6.173e-03
 Total CO2 (mol/kg) = 6.173e-03
 Temperature (°C) = 12.40
 Electrical balance (eq) = 8.828e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.33
 Iterations = 15 (146 overall)
 Total H = 1.110205e+02
 Total O = 5.554250e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	3.0698	0.1739
N(-3)/N(5)	6.5052	0.3686
O(-2)/O(0)	13.7787	0.7806

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	7.666e-08	6.629e-08	-7.115	-7.179	-0.063	(0)	
H+	6.472e-08	5.623e-08	-7.189	-7.250	-0.061	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	

C(4) 6.173e-03

HCO3-	5.279e-03	4.613e-03	-2.277	-2.336	-0.059	(0)
H2CO3	6.868e-04	6.868e-04	-3.163	-3.163	0.000	(0)
CaHCO3+	1.373e-04	1.204e-04	-3.862	-3.920	-0.057	(0)
MgHCO3+	4.603e-05	3.993e-05	-4.337	-4.399	-0.062	(0)
NaHCO3	8.392e-06	8.392e-06	-5.076	-5.076	0.000	(0)
CaCO3	7.071e-06	7.071e-06	-5.150	-5.150	0.000	(0)
CO3-2	5.202e-06	2.966e-06	-5.284	-5.528	-0.244	(0)
MgCO3	1.809e-06	1.809e-06	-5.742	-5.742	0.000	(0)
MnHCO3+	6.370e-07	5.555e-07	-6.196	-6.255	-0.059	(0)
FeHCO3+	3.786e-07	3.319e-07	-6.422	-6.479	-0.057	(0)
NaCO3-	2.300e-07	2.010e-07	-6.638	-6.697	-0.059	(0)
Ca2UO2(CO3)3	2.605e-08	2.618e-08	-7.584	-7.582	0.002	(0)
CaUO2(CO3)3-2	6.935e-09	3.954e-09	-8.159	-8.403	-0.244	(0)
UO2(CO3)3-4	1.605e-10	1.060e-11	-9.795	-10.975	-1.180	(0)
UO2(CO3)2-2	5.190e-11	2.631e-11	-10.285	-10.580	-0.295	(0)
MgUO2(CO3)3-2	2.179e-11	1.242e-11	-10.662	-10.906	-0.244	(0)
UO2CO3	5.505e-13	5.505e-13	-12.259	-12.259	0.000	(0)
(UO2)2CO3(OH)3-	7.956e-18	6.913e-18	-17.099	-17.160	-0.061	(0)
(UO2)3(CO3)6-6	5.234e-26	3.331e-28	-25.281	-27.477	-2.196	(0)

Ca 4.396e-03

Ca+2	3.508e-03	2.000e-03	-2.455	-2.699	-0.244	(0)
CaSO4	7.436e-04	7.436e-04	-3.129	-3.129	0.000	(0)
CaHCO3+	1.373e-04	1.204e-04	-3.862	-3.920	-0.057	(0)
CaCO3	7.071e-06	7.071e-06	-5.150	-5.150	0.000	(0)
Ca2UO2(CO3)3	2.605e-08	2.618e-08	-7.584	-7.582	0.002	(0)
CaNO3+	1.272e-08	1.073e-08	-7.896	-7.969	-0.074	(0)
CaUO2(CO3)3-2	6.935e-09	3.954e-09	-8.159	-8.403	-0.244	(0)
CaOH+	2.603e-09	2.282e-09	-8.584	-8.642	-0.057	(0)
CaNH3+2	2.993e-10	1.517e-10	-9.524	-9.819	-0.295	(0)
Ca(NH3)2+2	7.181e-18	3.641e-18	-17.144	-17.439	-0.295	(0)

Cl 1.601e-03

Cl-	1.601e-03	1.391e-03	-2.796	-2.857	-0.061	(0)
MnCl+	1.301e-08	1.135e-08	-7.886	-7.945	-0.059	(0)
MnCl2	2.230e-11	2.230e-11	-10.652	-10.652	0.000	(0)
MnCl3-	9.797e-15	8.544e-15	-14.009	-14.068	-0.059	(0)
FeCl+2	1.823e-17	1.055e-17	-16.739	-16.977	-0.238	(0)
FeCl2+	1.132e-19	9.869e-20	-18.946	-19.006	-0.059	(0)
UO2Cl+	1.007e-19	8.495e-20	-18.997	-19.071	-0.074	(0)
FeCl3	1.373e-23	1.373e-23	-22.862	-22.862	0.000	(0)
UO2Cl2	7.224e-24	7.260e-24	-23.141	-23.139	0.002	(0)
UCl+3	0.000e+00	0.000e+00	-40.508	-41.172	-0.664	(0)

Fe(2) 1.792e-05

Fe+2	1.462e-05	7.410e-06	-4.835	-5.130	-0.295	(0)
FeSO4	2.906e-06	2.906e-06	-5.537	-5.537	0.000	(0)
FeHCO3+	3.786e-07	3.319e-07	-6.422	-6.479	-0.057	(0)
FeOH+	2.242e-08	1.956e-08	-7.649	-7.709	-0.059	(0)
Fe(OH)2	8.930e-13	8.930e-13	-12.049	-12.049	0.000	(0)
Fe(OH)3-	5.135e-14	4.478e-14	-13.289	-13.349	-0.059	(0)

Fe(3) 3.585e-06

Fe(OH)2+	3.482e-06	3.043e-06	-5.458	-5.517	-0.059	(0)
Fe(OH)3	9.219e-08	9.219e-08	-7.035	-7.035	0.000	(0)
Fe(OH)4-	1.116e-08	9.749e-09	-7.953	-8.011	-0.059	(0)
FeOH+2	3.589e-11	2.076e-11	-10.445	-10.683	-0.238	(0)
FeSO4+	5.740e-15	5.006e-15	-14.241	-14.300	-0.059	(0)
Fe+3	1.338e-15	3.780e-16	-14.873	-15.422	-0.549	(0)
Fe(SO4)2-	2.590e-16	2.186e-16	-15.587	-15.660	-0.074	(0)
FeCl+2	1.823e-17	1.055e-17	-16.739	-16.977	-0.238	(0)
Fe2(OH)2+4	3.432e-19	2.267e-20	-18.464	-19.645	-1.180	(0)
FeCl2+	1.132e-19	9.869e-20	-18.946	-19.006	-0.059	(0)
FeHSeO3+2	4.439e-20	2.250e-20	-19.353	-19.648	-0.295	(0)
FeNO3+2	2.221e-20	1.126e-20	-19.653	-19.948	-0.295	(0)
Fe3(OH)4+5	6.078e-23	8.704e-25	-22.216	-24.060	-1.844	(0)
FeCl3	1.373e-23	1.373e-23	-22.862	-22.862	0.000	(0)

H(0) 3.204e-23

H2	1.602e-23	1.610e-23	-22.795	-22.793	0.002	(0)
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K 1.060e-04
K+ 1.047e-04 9.101e-05 -3.980 -4.041 -0.061 (0)
KSO4- 1.262e-06 1.103e-06 -5.899 -5.957 -0.059 (0)

Mg 1.915e-03
Mg+2 1.593e-03 9.081e-04 -2.798 -3.042 -0.244 (0)
MgSO4 2.745e-04 2.745e-04 -3.561 -3.561 0.000 (0)
MgHCO3+ 4.603e-05 3.993e-05 -4.337 -4.399 -0.062 (0)
MgCO3 1.809e-06 1.809e-06 -5.742 -5.742 0.000 (0)
MgOH+ 2.203e-08 1.936e-08 -7.657 -7.713 -0.056 (0)
MgUO2(CO3)3-2 2.179e-11 1.242e-11 -10.662 -10.906 -0.244 (0)

Mn(2) 1.525e-05
Mn+2 1.278e-05 6.480e-06 -4.893 -5.188 -0.295 (0)
MnSO4 1.818e-06 1.818e-06 -5.740 -5.740 0.000 (0)
MnHCO3+ 6.370e-07 5.555e-07 -6.196 -6.255 -0.059 (0)
MnCl+ 1.301e-08 1.135e-08 -7.886 -7.945 -0.059 (0)
MnOH+ 1.237e-09 1.079e-09 -8.908 -8.967 -0.059 (0)
MnCl2 2.230e-11 2.230e-11 -10.652 -10.652 0.000 (0)
MnNO3+ 1.876e-11 1.583e-11 -10.727 -10.800 -0.074 (0)
MnCl3- 9.797e-15 8.544e-15 -14.009 -14.068 -0.059 (0)
Mn(NO3)2 6.313e-17 6.313e-17 -16.200 -16.200 0.000 (0)
Mn(OH)3- 6.615e-19 5.769e-19 -18.179 -18.239 -0.059 (0)
MnSeO4 5.832e-22 5.832e-22 -21.234 -21.234 0.000 (0)
Mn(OH)4-2 5.764e-25 3.334e-25 -24.239 -24.477 -0.238 (0)
MnSe 9.615e-26 9.615e-26 -25.017 -25.017 0.000 (0)

Mn(3) 5.988e-29
Mn+3 5.988e-29 1.691e-29 -28.223 -28.772 -0.549 (0)

Mn(6) 0.000e+00
MnO4-2 0.000e+00 0.000e+00 -60.470 -60.708 -0.238 (0)

Mn(7) 0.000e+00
MnO4- 0.000e+00 0.000e+00 -68.278 -68.342 -0.064 (0)

Mo 1.116e-07
MoO4-2 1.116e-07 6.362e-08 -6.952 -7.196 -0.244 (0)
HMoO4- 5.909e-11 4.986e-11 -10.228 -10.302 -0.074 (0)
H2MoO4 4.658e-14 4.658e-14 -13.332 -13.332 0.000 (0)
Mo7O24-6 0.000e+00 0.000e+00 -50.966 -53.622 -2.655 (0)
HMo7O24-5 0.000e+00 0.000e+00 -52.718 -54.562 -1.844 (0)
H2Mo7O24-4 0.000e+00 0.000e+00 -55.873 -57.053 -1.180 (0)
H3Mo7O24-3 0.000e+00 0.000e+00 -60.378 -61.042 -0.664 (0)

N(-3) 7.075e-06
NH4+ 6.917e-06 5.944e-06 -5.160 -5.226 -0.066 (0)
NH4SO4- 1.345e-07 1.173e-07 -6.871 -6.931 -0.059 (0)
NH3 2.388e-08 2.388e-08 -7.622 -7.622 0.000 (0)
CaNH3+2 2.993e-10 1.517e-10 -9.524 -9.819 -0.295 (0)
Ca(NH3)2+2 7.181e-18 3.641e-18 -17.144 -17.439 -0.295 (0)

N(5) 1.787e-06
NO3- 1.774e-06 1.541e-06 -5.751 -5.812 -0.061 (0)
CaNO3+ 1.272e-08 1.073e-08 -7.896 -7.969 -0.074 (0)
MnNO3+ 1.876e-11 1.583e-11 -10.727 -10.800 -0.074 (0)
Mn(NO3)2 6.313e-17 6.313e-17 -16.200 -16.200 0.000 (0)
FeNO3+2 2.221e-20 1.126e-20 -19.653 -19.948 -0.295 (0)
UO2NO3+ 2.259e-22 1.906e-22 -21.646 -21.720 -0.074 (0)

Na 2.952e-03
Na+ 2.915e-03 2.533e-03 -2.535 -2.596 -0.061 (0)
NaSO4- 2.817e-05 2.461e-05 -4.550 -4.609 -0.059 (0)
NaHCO3 8.392e-06 8.392e-06 -5.076 -5.076 0.000 (0)
NaCO3- 2.300e-07 2.010e-07 -6.638 -6.697 -0.059 (0)

O(0) 5.005e-06
O2 2.503e-06 2.515e-06 -5.602 -5.599 0.002 (0)

S(6) 4.283e-03
SO4-2 3.230e-03 1.842e-03 -2.491 -2.735 -0.244 (0)
CaSO4 7.436e-04 7.436e-04 -3.129 -3.129 0.000 (0)
MgSO4 2.745e-04 2.745e-04 -3.561 -3.561 0.000 (0)
NaSO4- 2.817e-05 2.461e-05 -4.550 -4.609 -0.059 (0)
FeSO4 2.906e-06 2.906e-06 -5.537 -5.537 0.000 (0)
MnSO4 1.818e-06 1.818e-06 -5.740 -5.740 0.000 (0)
KSO4- 1.262e-06 1.103e-06 -5.899 -5.957 -0.059 (0)

NH4SO4-	1.345e-07	1.173e-07	-6.871	-6.931	-0.059	(0)
HSO4-	7.866e-09	6.842e-09	-8.104	-8.165	-0.061	(0)
FeSO4+	5.740e-15	5.006e-15	-14.241	-14.300	-0.059	(0)
Fe(SO4)2-	2.590e-16	2.186e-16	-15.587	-15.660	-0.074	(0)
UO2SO4	9.775e-17	9.775e-17	-16.010	-16.010	0.000	(0)
UO2(SO4)2-2	3.398e-18	1.723e-18	-17.469	-17.764	-0.295	(0)
U(SO4)2	4.028e-36	4.028e-36	-35.395	-35.395	0.000	(0)
USO4+2	8.475e-37	4.296e-37	-36.072	-36.367	-0.295	(0)
Se(-2)	2.401e-22					
HSe-	2.400e-22	2.025e-22	-21.620	-21.694	-0.074	(0)
MnSe	9.615e-26	9.615e-26	-25.017	-25.017	0.000	(0)
H2Se	8.334e-26	8.334e-26	-25.079	-25.079	0.000	(0)
Se-2	3.016e-30	1.529e-30	-29.521	-29.816	-0.295	(0)
Se(4)	4.615e-08					
HSeO3-	4.166e-08	3.515e-08	-7.380	-7.454	-0.074	(0)
SeO3-2	4.489e-09	2.276e-09	-8.348	-8.643	-0.295	(0)
H2SeO3	7.551e-13	7.551e-13	-12.122	-12.122	0.000	(0)
FeHSeO3+2	4.439e-20	2.250e-20	-19.353	-19.648	-0.295	(0)
Se(6)	7.531e-19					
SeO4-2	7.525e-19	4.290e-19	-18.124	-18.368	-0.244	(0)
MnSeO4	5.832e-22	5.832e-22	-21.234	-21.234	0.000	(0)
HSeO4-	9.515e-25	8.029e-25	-24.022	-24.095	-0.074	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-51.692	-52.356	-0.664	(0)
U(4)	1.387e-18					
U(OH)5-	1.383e-18	1.167e-18	-17.859	-17.933	-0.074	(0)
U(OH)4	3.391e-21	3.391e-21	-20.470	-20.470	0.000	(0)
U(OH)3+	9.674e-25	8.163e-25	-24.014	-24.088	-0.074	(0)
U(OH)2+2	6.040e-29	3.062e-29	-28.219	-28.514	-0.295	(0)
UOH+3	5.982e-34	1.297e-34	-33.223	-33.887	-0.664	(0)
U(SO4)2	4.028e-36	4.028e-36	-35.395	-35.395	0.000	(0)
USO4+2	8.475e-37	4.296e-37	-36.072	-36.367	-0.295	(0)
U+4	1.023e-39	0.000e+00	-38.990	-40.170	-1.180	(0)
UCl+3	0.000e+00	0.000e+00	-40.508	-41.172	-0.664	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-143.454	-149.429	-5.975	(0)
U(5)	1.161e-16					
UO2+	1.161e-16	9.799e-17	-15.935	-16.009	-0.074	(0)
U(6)	3.322e-08					
Ca2UO2(CO3)3	2.605e-08	2.618e-08	-7.584	-7.582	0.002	(0)
CaUO2(CO3)3-2	6.935e-09	3.954e-09	-8.159	-8.403	-0.244	(0)
UO2(CO3)3-4	1.605e-10	1.060e-11	-9.795	-10.975	-1.180	(0)
UO2(CO3)2-2	5.190e-11	2.631e-11	-10.285	-10.580	-0.295	(0)
MgUO2(CO3)3-2	2.179e-11	1.242e-11	-10.662	-10.906	-0.244	(0)
UO2(OH)2	7.628e-13	7.666e-13	-12.118	-12.115	0.002	(0)
UO2CO3	5.505e-13	5.505e-13	-12.259	-12.259	0.000	(0)
UO2(OH)3-	1.942e-14	1.688e-14	-13.712	-13.773	-0.061	(0)
UO2OH+	5.709e-16	4.817e-16	-15.243	-15.317	-0.074	(0)
UO2SO4	9.775e-17	9.775e-17	-16.010	-16.010	0.000	(0)
UO2+2	8.781e-17	5.006e-17	-16.056	-16.301	-0.244	(0)
(UO2)2CO3(OH)3-	7.956e-18	6.913e-18	-17.099	-17.160	-0.061	(0)
UO2(SO4)2-2	3.398e-18	1.723e-18	-17.469	-17.764	-0.295	(0)
UO2Cl+	1.007e-19	8.495e-20	-18.997	-19.071	-0.074	(0)
UO2(OH)4-2	8.200e-21	4.675e-21	-20.086	-20.330	-0.244	(0)
UO2NO3+	2.259e-22	1.906e-22	-21.646	-21.720	-0.074	(0)
UO2Cl2	7.224e-24	7.260e-24	-23.141	-23.139	0.002	(0)
(UO2)2(OH)2+2	1.979e-24	1.003e-24	-23.704	-23.999	-0.295	(0)
(UO2)3(CO3)6-6	5.234e-26	3.331e-28	-25.281	-27.477	-2.196	(0)
(UO2)2OH+3	3.095e-28	8.743e-29	-27.509	-28.058	-0.549	(0)
(UO2)3(OH)5+	1.003e-29	8.462e-30	-28.999	-29.073	-0.074	(0)
(UO2)3(OH)7-	7.205e-30	6.261e-30	-29.142	-29.203	-0.061	(0)
(UO2)3(OH)4+2	2.588e-32	1.475e-32	-31.587	-31.831	-0.244	(0)
(UO2)4(OH)7+	4.541e-37	3.946e-37	-36.343	-36.404	-0.061	(0)

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

Phase SI** log IAP log K(285 K, 1 atm)

(NH4)2SeO4 -29.27 -28.82 0.45 (NH4)2SeO4
 Anhydrite -1.13 -5.43 -4.30 CaSO4
 Aragonite -0.02 -8.23 -8.21 CaCO3
 Artinite -7.64 2.89 10.53 MgCO3:Mg(OH)2:3H2O
 Birnessite -15.26 2.83 18.09 MnO2
 Bixbyite -14.36 -14.04 0.32 Mn2O3
 Brucite -6.27 11.46 17.73 Mg(OH)2
 Calcite 0.19 -8.23 -8.42 CaCO3
 CaMoO4 -1.96 -9.90 -7.93 CaMoO4
 CaSeO3:2H2O -5.87 -2.90 2.96 CaSeO3:2H2O
 CaSeO4:2H2O -18.11 -21.07 -2.96 CaSeO4:2H2O
 CH4(g) -55.79 -98.83 -43.03 CH4
 CO2(g) -1.85 -20.03 -18.18 CO2
 Dolomite(disordered) -0.62 -16.80 -16.18 CaMg(CO3)2
 Dolomite(ordered) -0.01 -16.80 -16.78 CaMg(CO3)2
 Epsomite -3.56 -5.78 -2.22 MgSO4:7H2O
 Fe(OH)2 -4.19 9.37 13.56 Fe(OH)2
 Fe(OH)2.7Cl.3 6.34 3.30 -3.04 Fe(OH)2.7Cl.3
 Fe2(OH)4SeO3 -3.60 -2.05 1.55 Fe2(OH)4SeO3
 Fe2(SeO3)3:2H2O -10.83 -31.46 -20.63 Fe2(SeO3)3:2H2O
 Fe2(SO4)3 -37.19 -39.05 -1.86 Fe2(SO4)3
 Fe3(OH)8 1.80 22.02 20.22 Fe3(OH)8
 FeMoO4 -2.32 -12.33 -10.01 FeMoO4
 Ferrihydrite 2.57 6.33 3.76 Fe(OH)3
 Ferroselite -9.86 -28.82 -18.96 FeSe2
 FeSe -8.56 -19.57 -11.02 FeSe
 Goethite 5.37 6.33 0.96 FeOOH
 Gummite -10.10 -1.80 8.30 UO3
 Gypsum -0.82 -5.43 -4.62 CaSO4:2H2O
 H-Jarosite -5.17 -15.49 -10.32 (H3O)Fe3(SO4)2(OH)6
 H2MoO4 -8.44 -21.70 -13.26 H2MoO4
 H2Se(g) -24.10 -28.94 -4.84 H2Se
 Halite -7.03 -5.45 1.57 NaCl
 Hausmannite -16.65 47.63 64.28 Mn3O4
 Hematite 13.08 12.65 -0.42 Fe2O3
 Huntite -4.80 -33.94 -29.13 CaMg3(CO3)4
 Hydromagnesite -15.74 -22.82 -7.08 Mg5(CO3)4(OH)2:4H2O
 K-Jarosite 1.51 -12.28 -13.79 KFe3(SO4)2(OH)6
 K2MoO4 -18.57 -15.28 3.29 K2MoO4
 K2SeO4 -25.72 -26.45 -0.73 K2SeO4
 Lepidocrocite 4.96 6.33 1.37 FeOOH
 Lime -22.40 11.80 34.20 CaO
 Maghemite 6.27 12.65 6.39 Fe2O3
 Magnesioferrite 5.10 24.11 19.02 Fe2MgO4
 Magnesite -0.96 -8.57 -7.61 MgCO3
 Magnetite 17.01 22.02 5.01 Fe3O4
 Manganite -6.18 19.16 25.34 MnOOH
 Melanterite -5.50 -7.87 -2.37 FeSO4:7H2O
 Mg(OH)2(active) -7.34 11.46 18.79 Mg(OH)2
 MgMoO4 -8.39 -10.24 -1.85 MgMoO4
 MgSeO3:6H2O -6.26 -3.25 3.01 MgSeO3:6H2O
 MgSeO4:6H2O -20.21 -21.41 -1.20 MgSeO4:6H2O
 Mirabilite -6.20 -7.93 -1.73 Na2SO4:10H2O
 Mn2(SO4)3 -61.30 -65.75 -4.45 Mn2(SO4)3
 MnCl2:4H2O -13.70 -10.90 2.80 MnCl2:4H2O
 MnSe -23.89 -19.63 4.26 MnSe
 MnSeO3 -6.52 -5.39 1.13 MnSeO3
 MnSeO3:2H2O -6.31 -5.39 0.92 MnSeO3:2H2O
 MnSeO4:5H2O -21.51 -23.56 -2.05 MnSeO4:5H2O
 MnSO4 -11.01 -7.92 3.08 MnSO4
 MoO3 -13.70 -21.70 -8.00 MoO3
 Na-Jarosite -0.80 -10.83 -10.03 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -17.05 -34.09 -17.03 Na2Mo2O7
 Na2MoO4 -13.96 -12.39 1.57 Na2MoO4
 Na2MoO4:2H2O -13.61 -12.39 1.22 Na2MoO4:2H2O

Na2SeO3:5H2O -15.70 -5.40 10.30 Na2SeO3:5H2O
 Na2SeO4 -24.84 -23.56 1.28 Na2SeO4
 Natron -8.90 -10.72 -1.82 Na2CO3:10H2O
 Nesquehonite -4.09 -8.57 -4.48 MgCO3:3H2O
 Nsutite -14.68 2.83 17.50 MnO2
 O2(g) -48.11 39.40 87.51 O2
 Periclase -11.30 11.46 22.75 MgO
 Portlandite -12.00 11.80 23.80 Ca(OH)2
 Pyrochroite -6.63 9.31 15.94 Mn(OH)2
 Pyrolusite -14.47 29.01 43.48 MnO2
 Rhodochrosite -0.15 -10.72 -10.57 MnCO3
 Rutherfordine -7.35 -21.83 -14.48 UO2CO3
 Schoepite -8.18 -1.80 6.38 UO2(OH)2:H2O
 Semetal(am) -2.05 -9.24 -7.19 Se
 Semetal(hex) -1.41 -9.24 -7.83 Se
 SeO2 -14.82 -14.70 0.11 SeO2
 SeO3 -55.04 -32.87 22.18 SeO3
 Siderite -0.54 -10.66 -10.12 FeCO3
 Thenardite -8.32 -7.93 0.39 Na2SO4
 Thermonatrite -11.44 -10.72 0.72 Na2CO3:H2O
 U3O8 -18.95 5.89 24.84 U3O8
 U4O9 -25.26 -24.98 0.28 U4O9
 UO2(am) -12.95 -11.17 1.78 UO2
 UO2(NO3)2 -40.72 -27.92 12.79 UO2(NO3)2
 UO2(NO3)2:2H2O -32.97 -27.92 5.05 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -31.39 -27.93 3.46 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -29.81 -27.93 1.89 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -7.85 -1.80 6.05 UO2(OH)2
 UO2SeO4:4H2O -32.42 -34.67 -2.25 UO2SeO4:4H2O
 UO3 -10.13 -1.80 8.33 UO3
 Uraninite -7.10 -11.17 -4.07 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 9. SAG2-4

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

Elements	Molality	Moles
Alkalinity	4.741e-03	4.741e-03
Ca	3.821e-03	3.821e-03
Cl	1.742e-03	1.742e-03
Fe(2)	5.843e-05	5.843e-05
Fe(3)	9.679e-06	9.679e-06
K	1.134e-04	1.134e-04
Mg	1.985e-03	1.985e-03
Mn	3.480e-05	3.480e-05
Mo	1.826e-07	1.826e-07
N(-3)	5.617e-05	5.617e-05
N(5)	1.429e-06	1.429e-06
Na	3.605e-03	3.605e-03
O(0)	4.380e-06	4.380e-06
S(-2)	8.117e-07	8.117e-07
S(6)	4.543e-03	4.543e-03
Se	1.268e-09	1.268e-09
U	2.044e-08	2.044e-08

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

pH = 7.560
 pe = 0.800
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.154e-02
 Mass of water (kg) = 1.000e+00

Total carbon (mol/kg) = 5.002e-03
 Total CO2 (mol/kg) = 5.002e-03
 Temperature (°C) = 12.90
 Electrical balance (eq) = 1.340e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.05
 Iterations = 20 (166 overall)
 Total H = 1.110192e+02
 Total O = 5.554004e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	2.3415	0.1329
N(-3)/N(5)	5.9621	0.3384
O(-2)/O(0)	13.4158	0.7614
S(-2)/S(6)	-3.7906	-0.2151

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.630e-07	1.410e-07	-6.788	-6.851	-0.063	(0)	
H+	3.168e-08	2.754e-08	-7.499	-7.560	-0.061	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	
C(4)	5.002e-03						
HCO3-	4.536e-03	3.966e-03	-2.343	-2.402	-0.058	(0)	
H2CO3	2.872e-04	2.872e-04	-3.542	-3.542	0.000	(0)	
CaHCO3+	1.030e-04	9.034e-05	-3.987	-4.044	-0.057	(0)	
MgHCO3+	4.079e-05	3.540e-05	-4.389	-4.451	-0.062	(0)	
CaCO3	1.092e-05	1.092e-05	-4.962	-4.962	0.000	(0)	
CO3-2	9.209e-06	5.262e-06	-5.036	-5.279	-0.243	(0)	
NaHCO3	8.722e-06	8.722e-06	-5.059	-5.059	0.000	(0)	
MgCO3	3.331e-06	3.331e-06	-5.477	-5.477	0.000	(0)	
MnHCO3+	1.250e-06	1.091e-06	-5.903	-5.962	-0.059	(0)	
FeHCO3+	1.061e-06	9.307e-07	-5.974	-6.031	-0.057	(0)	
NaCO3-	4.907e-07	4.290e-07	-6.309	-6.367	-0.058	(0)	
Ca2UO2(CO3)3	1.549e-08	1.557e-08	-7.810	-7.808	0.002	(0)	
CaUO2(CO3)3-2	4.781e-09	2.732e-09	-8.320	-8.564	-0.243	(0)	
UO2(CO3)3-4	1.234e-10	8.263e-12	-9.909	-11.083	-1.174	(0)	
UO2(CO3)2-2	2.369e-11	1.205e-11	-10.625	-10.919	-0.294	(0)	
MgUO2(CO3)3-2	1.795e-11	1.026e-11	-10.746	-10.989	-0.243	(0)	
UO2CO3	1.409e-13	1.409e-13	-12.851	-12.851	0.000	(0)	
(UO2)2CO3(OH)3-	2.457e-18	2.136e-18	-17.610	-17.670	-0.061	(0)	
(UO2)3(CO3)6-6	4.459e-27	2.896e-29	-26.351	-28.538	-2.187	(0)	
Ca	3.821e-03						
Ca+2	3.012e-03	1.721e-03	-2.521	-2.764	-0.243	(0)	
CaSO4	6.958e-04	6.958e-04	-3.158	-3.158	0.000	(0)	
CaHCO3+	1.030e-04	9.034e-05	-3.987	-4.044	-0.057	(0)	
CaCO3	1.092e-05	1.092e-05	-4.962	-4.962	0.000	(0)	
Ca2UO2(CO3)3	1.549e-08	1.557e-08	-7.810	-7.808	0.002	(0)	
CaNO3+	8.727e-09	7.370e-09	-8.059	-8.133	-0.073	(0)	
CaOH+	4.792e-09	4.203e-09	-8.319	-8.376	-0.057	(0)	
CaUO2(CO3)3-2	4.781e-09	2.732e-09	-8.320	-8.564	-0.243	(0)	
CaNH3+2	4.141e-09	2.107e-09	-8.383	-8.676	-0.294	(0)	
Ca(NH3)2+2	1.603e-15	8.155e-16	-14.795	-15.089	-0.294	(0)	
Cl	1.742e-03						
Cl-	1.742e-03	1.515e-03	-2.759	-2.820	-0.061	(0)	
MnCl+	3.225e-08	2.814e-08	-7.492	-7.551	-0.059	(0)	
MnCl2	6.020e-11	6.020e-11	-10.220	-10.220	0.000	(0)	
MnCl3-	2.878e-14	2.511e-14	-13.541	-13.600	-0.059	(0)	
FeCl+2	1.254e-17	7.271e-18	-16.902	-17.138	-0.237	(0)	
FeCl2+	8.347e-20	7.284e-20	-19.078	-19.138	-0.059	(0)	
UO2Cl+	1.594e-20	1.346e-20	-19.798	-19.871	-0.073	(0)	
FeCl3	1.103e-23	1.103e-23	-22.957	-22.957	0.000	(0)	

UO2Cl2	1.232e-24	1.238e-24	-23.910	-23.907	0.002	(0)
UCl+3	9.782e-40	2.138e-40	-39.010	-39.670	-0.660	(0)
Fe(2)	5.843e-05					
Fe+2	4.701e-05	2.391e-05	-4.328	-4.621	-0.294	(0)
FeSO4	1.020e-05	1.020e-05	-4.991	-4.991	0.000	(0)
FeHCO3+	1.061e-06	9.307e-07	-5.974	-6.031	-0.057	(0)
FeOH+	1.539e-07	1.343e-07	-6.813	-6.872	-0.059	(0)
Fe(HS)2	5.126e-09	5.126e-09	-8.290	-8.290	0.000	(0)
Fe(OH)2	1.312e-11	1.312e-11	-10.882	-10.882	0.000	(0)
Fe(OH)3-	1.547e-12	1.350e-12	-11.810	-11.870	-0.059	(0)
Fe(HS)3-	3.242e-13	2.738e-13	-12.489	-12.563	-0.073	(0)
Fe(3)	9.679e-06					
Fe(OH)2+	9.031e-06	7.897e-06	-5.044	-5.103	-0.058	(0)
Fe(OH)3	5.273e-07	5.273e-07	-6.278	-6.278	0.000	(0)
Fe(OH)4-	1.206e-07	1.055e-07	-6.919	-6.977	-0.058	(0)
FeOH+2	4.694e-11	2.721e-11	-10.328	-10.565	-0.237	(0)
FeSO4+	3.935e-15	3.434e-15	-14.405	-14.464	-0.059	(0)
Fe+3	8.291e-16	2.354e-16	-15.081	-15.628	-0.547	(0)
Fe(SO4)2-	1.912e-16	1.615e-16	-15.719	-15.792	-0.073	(0)
FeCl+2	1.254e-17	7.271e-18	-16.902	-17.138	-0.237	(0)
Fe2(OH)2+4	5.706e-19	3.821e-20	-18.244	-19.418	-1.174	(0)
FeCl2+	8.347e-20	7.284e-20	-19.078	-19.138	-0.059	(0)
FeNO3+2	1.074e-20	5.466e-21	-19.969	-20.262	-0.294	(0)
FeHSeO3+2	7.002e-22	3.562e-22	-21.155	-21.448	-0.294	(0)
Fe3(OH)4+5	2.617e-22	3.830e-24	-21.582	-23.417	-1.835	(0)
FeCl3	1.103e-23	1.103e-23	-22.957	-22.957	0.000	(0)
H(0)	3.044e-20					
H2	1.522e-20	1.529e-20	-19.818	-19.815	0.002	(0)
K	1.134e-04					
K+	1.120e-04	9.734e-05	-3.951	-4.012	-0.061	(0)
KSO4-	1.464e-06	1.280e-06	-5.834	-5.893	-0.058	(0)
Mg	1.985e-03					
Mg+2	1.634e-03	9.339e-04	-2.787	-3.030	-0.243	(0)
MgSO4	3.066e-04	3.066e-04	-3.513	-3.513	0.000	(0)
MgHCO3+	4.079e-05	3.540e-05	-4.389	-4.451	-0.062	(0)
MgCO3	3.331e-06	3.331e-06	-5.477	-5.477	0.000	(0)
MgOH+	4.860e-08	4.272e-08	-7.313	-7.369	-0.056	(0)
MgUO2(CO3)3-2	1.795e-11	1.026e-11	-10.746	-10.989	-0.243	(0)
Mn(2)	3.480e-05					
Mn+2	2.901e-05	1.476e-05	-4.537	-4.831	-0.294	(0)
MnSO4	4.506e-06	4.506e-06	-5.346	-5.346	0.000	(0)
MnHCO3+	1.250e-06	1.091e-06	-5.903	-5.962	-0.059	(0)
MnCl+	3.225e-08	2.814e-08	-7.492	-7.551	-0.059	(0)
MnOH+	5.990e-09	5.227e-09	-8.223	-8.282	-0.059	(0)
MnCl2	6.020e-11	6.020e-11	-10.220	-10.220	0.000	(0)
MnNO3+	3.420e-11	2.889e-11	-10.466	-10.539	-0.073	(0)
MnCl3-	2.878e-14	2.511e-14	-13.541	-13.600	-0.059	(0)
Mn(NO3)2	9.219e-17	9.219e-17	-16.035	-16.035	0.000	(0)
Mn(OH)3-	1.282e-17	1.118e-17	-16.892	-16.951	-0.059	(0)
MnSe	9.719e-18	9.719e-18	-17.012	-17.012	0.000	(0)
Mn(OH)4-2	2.276e-23	1.319e-23	-22.643	-22.880	-0.237	(0)
MnSeO4	8.304e-26	8.304e-26	-25.081	-25.081	0.000	(0)
Mn(3)	2.328e-30					
Mn+3	2.328e-30	6.609e-31	-29.633	-30.180	-0.547	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-64.606	-64.843	-0.237	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-74.178	-74.242	-0.064	(0)
Mo	1.826e-07					
MoO4-2	1.825e-07	1.043e-07	-6.739	-6.982	-0.243	(0)
HMoO4-	4.812e-11	4.064e-11	-10.318	-10.391	-0.073	(0)
H2MoO4	1.797e-14	1.797e-14	-13.745	-13.745	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-52.030	-54.672	-2.642	(0)
HMo7O24-5	0.000e+00	0.000e+00	-54.084	-55.919	-1.835	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-57.545	-58.719	-1.174	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-62.358	-63.018	-0.660	(0)

N(-3) 5.617e-05
 NH4+ 5.462e-05 4.697e-05 -4.263 -4.328 -0.066 (0)
 NH4SO4- 1.149e-06 1.003e-06 -5.940 -5.999 -0.059 (0)
 NH3 4.004e-07 4.004e-07 -6.398 -6.398 0.000 (0)
 CaNH3+2 4.141e-09 2.107e-09 -8.383 -8.676 -0.294 (0)
 Ca(NH3)2+2 1.603e-15 8.155e-16 -14.795 -15.089 -0.294 (0)
 N(5) 1.429e-06
 NO3- 1.421e-06 1.235e-06 -5.848 -5.908 -0.061 (0)
 CaNO3+ 8.727e-09 7.370e-09 -8.059 -8.133 -0.073 (0)
 MnNO3+ 3.420e-11 2.889e-11 -10.466 -10.539 -0.073 (0)
 Mn(NO3)2 9.219e-17 9.219e-17 -16.035 -16.035 0.000 (0)
 FeNO3+2 1.074e-20 5.466e-21 -19.969 -20.262 -0.294 (0)
 UO2NO3+ 2.578e-23 2.177e-23 -22.589 -22.662 -0.073 (0)
 Na 3.605e-03
 Na+ 3.559e-03 3.094e-03 -2.449 -2.509 -0.061 (0)
 NaSO4- 3.722e-05 3.254e-05 -4.429 -4.488 -0.058 (0)
 NaHCO3 8.722e-06 8.722e-06 -5.059 -5.059 0.000 (0)
 NaCO3- 4.907e-07 4.290e-07 -6.309 -6.367 -0.058 (0)
 O(0) 4.380e-06
 O2 2.190e-06 2.201e-06 -5.660 -5.657 0.002 (0)
 S(-2) 8.117e-07
 HS- 5.807e-07 4.904e-07 -6.236 -6.309 -0.073 (0)
 H2S 2.059e-07 2.059e-07 -6.686 -6.686 0.000 (0)
 S5-2 7.950e-09 4.044e-09 -8.100 -8.393 -0.294 (0)
 Fe(HS)2 5.126e-09 5.126e-09 -8.290 -8.290 0.000 (0)
 S6-2 4.604e-09 2.342e-09 -8.337 -8.630 -0.294 (0)
 S4-2 1.959e-09 9.966e-10 -8.708 -9.001 -0.294 (0)
 S3-2 2.915e-10 1.483e-10 -9.535 -9.829 -0.294 (0)
 S2-2 2.615e-11 1.330e-11 -10.583 -10.876 -0.294 (0)
 Fe(HS)3- 3.242e-13 2.738e-13 -12.489 -12.563 -0.073 (0)
 S-2 6.627e-17 3.841e-17 -16.179 -16.416 -0.237 (0)
 S(6) 4.543e-03
 SO4-2 3.486e-03 1.992e-03 -2.458 -2.701 -0.243 (0)
 CaSO4 6.958e-04 6.958e-04 -3.158 -3.158 0.000 (0)
 MgSO4 3.066e-04 3.066e-04 -3.513 -3.513 0.000 (0)
 NaSO4- 3.722e-05 3.254e-05 -4.429 -4.488 -0.058 (0)
 FeSO4 1.020e-05 1.020e-05 -4.991 -4.991 0.000 (0)
 MnSO4 4.506e-06 4.506e-06 -5.346 -5.346 0.000 (0)
 KSO4- 1.464e-06 1.280e-06 -5.834 -5.893 -0.058 (0)
 NH4SO4- 1.149e-06 1.003e-06 -5.940 -5.999 -0.059 (0)
 HSO4- 4.233e-09 3.684e-09 -8.373 -8.434 -0.060 (0)
 FeSO4+ 3.935e-15 3.434e-15 -14.405 -14.464 -0.059 (0)
 Fe(SO4)2- 1.912e-16 1.615e-16 -15.719 -15.792 -0.073 (0)
 UO2SO4 1.543e-17 1.543e-17 -16.812 -16.812 0.000 (0)
 UO2(SO4)2-2 5.859e-19 2.981e-19 -18.232 -18.526 -0.294 (0)
 U(SO4)2 1.431e-34 1.431e-34 -33.845 -33.845 0.000 (0)
 USO4+2 2.723e-35 1.385e-35 -34.565 -34.859 -0.294 (0)
 Se(-2) 5.223e-15
 HSe- 5.212e-15 4.402e-15 -14.283 -14.356 -0.073 (0)
 MnSe 9.719e-18 9.719e-18 -17.012 -17.012 0.000 (0)
 H2Se 8.896e-19 8.896e-19 -18.051 -18.051 0.000 (0)
 Se-2 1.382e-22 7.032e-23 -21.859 -22.153 -0.294 (0)
 Se(4) 1.268e-09
 HSeO3- 1.039e-09 8.774e-10 -8.983 -9.057 -0.073 (0)
 SeO3-2 2.288e-10 1.164e-10 -9.640 -9.934 -0.294 (0)
 H2SeO3 9.274e-15 9.274e-15 -14.033 -14.033 0.000 (0)
 FeHSeO3+2 7.002e-22 3.562e-22 -21.155 -21.448 -0.294 (0)
 Se(6) 4.655e-23
 SeO4-2 4.646e-23 2.655e-23 -22.333 -22.576 -0.243 (0)
 MnSeO4 8.304e-26 8.304e-26 -25.081 -25.081 0.000 (0)
 HSeO4- 2.931e-29 2.475e-29 -28.533 -28.606 -0.073 (0)
 U(3) 0.000e+00
 U+3 0.000e+00 0.000e+00 -48.391 -49.051 -0.660 (0)
 U(4) 1.583e-15
 U(OH)5- 1.582e-15 1.336e-15 -14.801 -14.874 -0.073 (0)
 U(OH)4 1.884e-18 1.884e-18 -17.725 -17.725 0.000 (0)

U(OH)3+ 2.614e-22 2.207e-22 -21.583 -21.656 -0.073 (0)
 U(OH)2+2 7.851e-27 3.994e-27 -26.105 -26.399 -0.294 (0)
 UOH+3 3.719e-32 8.128e-33 -31.430 -32.090 -0.660 (0)
 U(SO4)2 1.431e-34 1.431e-34 -33.845 -33.845 0.000 (0)
 USO4+2 2.723e-35 1.385e-35 -34.565 -34.859 -0.294 (0)
 U+4 2.989e-38 2.002e-39 -37.524 -38.699 -1.174 (0)
 UCl+3 9.782e-40 2.138e-40 -39.010 -39.670 -0.660 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -130.004 -135.949 -5.944 (0)
 U(5) 1.042e-15
 UO2+ 1.042e-15 8.801e-16 -14.982 -15.055 -0.073 (0)
 U(6) 2.044e-08
 Ca2UO2(CO3)3 1.549e-08 1.557e-08 -7.810 -7.808 0.002 (0)
 CaUO2(CO3)3-2 4.781e-09 2.732e-09 -8.320 -8.564 -0.243 (0)
 UO2(CO3)3-4 1.234e-10 8.263e-12 -9.909 -11.083 -1.174 (0)
 UO2(CO3)2-2 2.369e-11 1.205e-11 -10.625 -10.919 -0.294 (0)
 MgUO2(CO3)3-2 1.795e-11 1.026e-11 -10.746 -10.989 -0.243 (0)
 UO2(OH)2 4.573e-13 4.596e-13 -12.340 -12.338 0.002 (0)
 UO2CO3 1.409e-13 1.409e-13 -12.851 -12.851 0.000 (0)
 UO2(OH)3- 2.376e-14 2.066e-14 -13.624 -13.685 -0.061 (0)
 UO2OH+ 1.735e-16 1.465e-16 -15.761 -15.834 -0.073 (0)
 UO2SO4 1.543e-17 1.543e-17 -16.812 -16.812 0.000 (0)
 UO2+2 1.260e-17 7.199e-18 -16.900 -17.143 -0.243 (0)
 (UO2)2CO3(OH)3- 2.457e-18 2.136e-18 -17.610 -17.670 -0.061 (0)
 UO2(SO4)2-2 5.859e-19 2.981e-19 -18.232 -18.526 -0.294 (0)
 UO2(OH)4-2 2.045e-20 1.168e-20 -19.689 -19.932 -0.243 (0)
 UO2Cl+ 1.594e-20 1.346e-20 -19.798 -19.871 -0.073 (0)
 UO2NO3+ 2.578e-23 2.177e-23 -22.589 -22.662 -0.073 (0)
 UO2Cl2 1.232e-24 1.238e-24 -23.910 -23.907 0.002 (0)
 (UO2)2(OH)2+2 1.753e-25 8.920e-26 -24.756 -25.050 -0.294 (0)
 (UO2)3(CO3)6-6 4.459e-27 2.896e-29 -26.351 -28.538 -2.187 (0)
 (UO2)2OH+3 1.300e-29 3.692e-30 -28.886 -29.433 -0.547 (0)
 (UO2)3(OH)7- 3.168e-30 2.754e-30 -29.499 -29.560 -0.061 (0)
 (UO2)3(OH)5+ 1.145e-30 9.669e-31 -29.941 -30.015 -0.073 (0)
 (UO2)3(OH)4+2 1.334e-33 7.625e-34 -32.875 -33.118 -0.243 (0)
 (UO2)4(OH)7+ 2.871e-38 2.496e-38 -37.542 -37.603 -0.061 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-31.68	-31.23	0.45 (NH4)2SeO4
Anhydrite	-1.16	-5.46	-4.31 CaSO4
Aragonite	0.17	-8.04	-8.21 CaCO3
Artinite	-6.71	3.78	10.49 MgCO3:Mg(OH)2:3H2O
Birnessite	-17.23	0.86	18.09 MnO2
Bixbyite	-15.28	-15.00	0.28 Mn2O3
Brucite	-5.60	12.09	17.69 Mg(OH)2
Calcite	0.38	-8.04	-8.42 CaCO3
CaMoO4	-1.81	-9.75	-7.94 CaMoO4
CaSeO3:2H2O	-7.22	-4.26	2.96 CaSeO3:2H2O
CaSeO4:2H2O	-22.38	-25.34	-2.96 CaSeO4:2H2O
CH4(g)	-44.33	-87.28	-42.95 CH4
CO2(g)	-2.22	-20.40	-18.18 CO2
Dolomite(disordered)	-0.16	-16.35	-16.20 CaMg(CO3)2
Dolomite(ordered)	0.45	-16.35	-16.80 CaMg(CO3)2
Epsomite	-3.52	-5.73	-2.21 MgSO4:7H2O
Fe(OH)2	-3.07	10.50	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	6.98	3.94	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-4.07	-2.51	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-15.12	-35.75	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-37.42	-39.36	-1.94 Fe2(SO4)3
Fe3(OH)8	4.38	24.60	20.22 Fe3(OH)8
FeMoO4	-1.59	-11.60	-10.01 FeMoO4
Ferrihydrite	3.32	7.05	3.73 Fe(OH)3
Ferroselite	2.33	-16.61	-18.95 FeSe2
FeS(ppt)	-0.50	-3.37	-2.87 FeS

FeSe	-0.40	-11.42	-11.02	FeSe
Goethite	6.11	7.05	0.94	FeOOH
Greigite	14.16	-30.88	-45.03	Fe ₃ S ₄
Gummite	-10.30	-2.02	8.27	UO ₃
Gypsum	-0.85	-5.47	-4.62	CaSO ₄ :2H ₂ O
H-Jarosite	-4.10	-14.49	-10.39	(H ₃ O)Fe ₃ (SO ₄) ₂ (OH) ₆
H ₂ MoO ₄	-8.86	-22.10	-13.24	H ₂ MoO ₄
H ₂ S(g)	-5.86	-13.87	-8.01	H ₂ S
H ₂ Se(g)	-17.07	-21.92	-4.85	H ₂ Se
Halite	-6.90	-5.33	1.58	NaCl
Hausmannite	-16.56	47.59	64.15	Mn ₃ O ₄
Hematite	14.57	14.10	-0.46	Fe ₂ O ₃
Huntite	-3.80	-32.97	-29.17	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-14.00	-21.14	-7.15	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
K-Jarosite	2.89	-10.94	-13.83	KFe ₃ (SO ₄) ₂ (OH) ₆
K ₂ MoO ₄	-18.29	-15.01	3.29	K ₂ MoO ₄
K ₂ SeO ₄	-29.87	-30.60	-0.73	K ₂ SeO ₄
Lepidocrocite	5.68	7.05	1.37	FeOOH
Lime	-21.78	12.36	34.14	CaO
Mackinawite	0.23	-3.37	-3.60	FeS
Maghemite	7.72	14.10	6.39	Fe ₂ O ₃
Magnesianoferrite	7.27	26.19	18.93	Fe ₂ MgO ₄
Magnesite	-0.70	-8.31	-7.61	MgCO ₃
Magnetite	19.65	24.60	4.95	Fe ₃ O ₄
Manganite	-6.69	18.65	25.34	MnOOH
Melanterite	-4.96	-7.32	-2.36	FeSO ₄ :7H ₂ O
Mg(OH) ₂ (active)	-6.70	12.09	18.79	Mg(OH) ₂
MgMoO ₄	-8.16	-10.01	-1.85	MgMoO ₄
MgSeO ₃ :6H ₂ O	-7.54	-4.53	3.02	MgSeO ₃ :6H ₂ O
MgSeO ₄ :6H ₂ O	-24.41	-25.61	-1.20	MgSeO ₄ :6H ₂ O
Mirabilite	-6.02	-7.72	-1.70	Na ₂ SO ₄ :10H ₂ O
Mn ₂ (SO ₄) ₃	-63.96	-68.46	-4.50	Mn ₂ (SO ₄) ₃
MnCl ₂ :4H ₂ O	-13.27	-10.47	2.80	MnCl ₂ :4H ₂ O
MnS(grn)	-3.99	-3.58	0.41	MnS
MnS(pnk)	-6.92	-3.58	3.34	MnS
MnSe	-15.85	-11.63	4.23	MnSe
MnSeO ₃	-7.46	-6.33	1.13	MnSeO ₃
MnSeO ₃ :2H ₂ O	-7.25	-6.33	0.92	MnSeO ₃ :2H ₂ O
MnSeO ₄ :5H ₂ O	-25.36	-27.41	-2.05	MnSeO ₄ :5H ₂ O
MnSO ₄	-10.60	-7.53	3.06	MnSO ₄
MoO ₃	-14.10	-22.10	-8.00	MoO ₃
MoS ₂	6.58	-66.56	-73.14	MoS ₂
Na-Jarosite	0.64	-9.44	-10.08	NaFe ₃ (SO ₄) ₂ (OH) ₆
Na ₂ Mo ₂ O ₇	-17.09	-34.10	-17.01	Na ₂ Mo ₂ O ₇
Na ₂ MoO ₄	-13.56	-12.00	1.56	Na ₂ MoO ₄
Na ₂ MoO ₄ :2H ₂ O	-13.22	-12.00	1.22	Na ₂ MoO ₄ :2H ₂ O
Na ₂ SeO ₃ :5H ₂ O	-16.82	-6.52	10.30	Na ₂ SeO ₃ :5H ₂ O
Na ₂ SeO ₄	-28.87	-27.59	1.28	Na ₂ SeO ₄
Natron	-8.50	-10.30	-1.80	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-3.82	-8.31	-4.49	MgCO ₃ :3H ₂ O
Nsutite	-16.64	0.86	17.50	MnO ₂
O ₂ (g)	-53.89	33.44	87.33	O ₂
Periclase	-10.61	12.09	22.70	MgO
Portlandite	-11.40	12.36	23.76	Ca(OH) ₂
Pyrite	18.36	-0.52	-18.88	FeS ₂
Pyrochroite	-5.62	10.29	15.91	Mn(OH) ₂
Pyrolusite	-16.39	27.01	43.40	MnO ₂
Rhodochrosite	0.46	-10.11	-10.57	MnCO ₃
Rutherfordine	-7.94	-22.42	-14.48	UO ₂ CO ₃
Schoepite	-8.39	-2.02	6.36	UO ₂ (OH) ₂ :H ₂ O
Semetal(am)	1.99	-5.20	-7.19	Se
Semetal(hex)	2.63	-5.20	-7.83	Se
SeO ₂	-16.73	-16.62	0.11	SeO ₂
SeO ₃	-59.82	-37.70	22.13	SeO ₃
Siderite	0.22	-9.90	-10.12	FeCO ₃
Sulfur	4.87	2.85	-2.02	S

Thenardite -8.11 -7.72 0.39 Na2SO4
 Thermonatrite -11.01 -10.30 0.71 Na2CO3:H2O
 U3O8 -16.62 8.06 24.68 U3O8
 U4O9 -17.26 -17.12 0.14 U4O9
 UO2(am) -10.21 -8.46 1.75 UO2
 UO2(NO3)2 -41.72 -28.96 12.77 UO2(NO3)2
 UO2(NO3)2:2H2O -34.00 -28.96 5.04 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -32.42 -28.96 3.46 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -30.85 -28.96 1.89 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -8.06 -2.02 6.03 UO2(OH)2
 UO2SeO4:4H2O -37.47 -39.72 -2.25 UO2SeO4:4H2O
 UO3 -10.32 -2.02 8.30 UO3
 Uraninite -4.37 -8.46 -4.09 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 10. SAG2-5

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

Elements	Molality	Moles
Alkalinity	4.281e-03	4.281e-03
Ca	4.871e-03	4.871e-03
Cl	1.570e-03	1.570e-03
Fe(2)	3.801e-05	3.801e-05
Fe(3)	1.040e-05	1.040e-05
K	1.058e-04	1.058e-04
Mg	2.002e-03	2.002e-03
Mn	8.164e-05	8.164e-05
Mo	1.430e-07	1.430e-07
N(-3)	1.544e-05	1.544e-05
N(5)	1.430e-06	1.430e-06
Na	2.896e-03	2.896e-03
O(0)	8.760e-06	8.760e-06
S(6)	6.180e-03	6.180e-03
Se	1.902e-09	1.902e-09
U	2.448e-09	2.448e-09

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

pH = 7.490
 pe = 1.400
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.448e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 4.561e-03
 Total CO2 (mol/kg) = 4.561e-03
 Temperature (°C) = 13.20
 Electrical balance (eq) = -1.200e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -4.15
 Iterations = 20 (186 overall)
 Total H = 1.110186e+02
 Total O = 5.554527e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	2.7291	0.1551
N(-3)/N(5)	6.1013	0.3466
O(-2)/O(0)	13.5381	0.7692

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.433e-07	1.230e-07	-6.844	-6.910	-0.066	(0)	
H+	3.750e-08	3.236e-08	-7.426	-7.490	-0.064	0.00	
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.03	
C(4)	4.561e-03						
HCO3-	4.085e-03	3.547e-03	-2.389	-2.450	-0.061	(0)	
H2CO3	3.006e-04	3.006e-04	-3.522	-3.522	0.000	(0)	
CaHCO3+	1.109e-04	9.657e-05	-3.955	-4.015	-0.060	(0)	
MgHCO3+	3.474e-05	2.991e-05	-4.459	-4.524	-0.065	(0)	
CaCO3	9.984e-06	9.984e-06	-5.001	-5.001	0.000	(0)	
CO3-2	7.270e-06	4.032e-06	-5.138	-5.395	-0.256	(0)	
NaHCO3	6.165e-06	6.165e-06	-5.210	-5.210	0.000	(0)	
MnHCO3+	2.463e-06	2.134e-06	-5.608	-5.671	-0.062	(0)	
MgCO3	2.419e-06	2.419e-06	-5.616	-5.616	0.000	(0)	
FeHCO3+	5.749e-07	5.008e-07	-6.240	-6.300	-0.060	(0)	
NaCO3-	2.983e-07	2.590e-07	-6.525	-6.587	-0.061	(0)	
Ca2UO2(CO3)3	1.916e-09	1.927e-09	-8.718	-8.715	0.002	(0)	
CaUO2(CO3)3-2	5.147e-10	2.854e-10	-9.288	-9.544	-0.256	(0)	
UO2(CO3)3-4	1.281e-11	7.160e-13	-10.893	-12.145	-1.253	(0)	
UO2(CO3)2-2	2.873e-12	1.397e-12	-11.542	-11.855	-0.313	(0)	
MgUO2(CO3)3-2	1.538e-12	8.531e-13	-11.813	-12.069	-0.256	(0)	
UO2CO3	2.120e-14	2.120e-14	-13.674	-13.674	0.000	(0)	
(UO2)2CO3(OH)3-	4.466e-20	3.854e-20	-19.350	-19.414	-0.064	(0)	
(UO2)3(CO3)6-6	8.568e-30	4.249e-32	-29.067	-31.372	-2.305	(0)	
Ca	4.871e-03						
Ca+2	3.676e-03	2.039e-03	-2.435	-2.691	-0.256	(0)	
CaSO4	1.074e-03	1.074e-03	-2.969	-2.969	0.000	(0)	
CaHCO3+	1.109e-04	9.657e-05	-3.955	-4.015	-0.060	(0)	
CaCO3	9.984e-06	9.984e-06	-5.001	-5.001	0.000	(0)	
CaNO3+	1.034e-08	8.636e-09	-7.985	-8.064	-0.078	(0)	
CaOH+	5.003e-09	4.359e-09	-8.301	-8.361	-0.060	(0)	
Ca2UO2(CO3)3	1.916e-09	1.927e-09	-8.718	-8.715	0.002	(0)	
CaNH3+2	1.184e-09	5.757e-10	-8.927	-9.240	-0.313	(0)	
CaUO2(CO3)3-2	5.147e-10	2.854e-10	-9.288	-9.544	-0.256	(0)	
Ca(NH3)2+2	1.057e-16	5.140e-17	-15.976	-16.289	-0.313	(0)	
Cl	1.570e-03						
Cl-	1.570e-03	1.355e-03	-2.804	-2.868	-0.064	(0)	
MnCl+	6.345e-08	5.497e-08	-7.198	-7.260	-0.062	(0)	
MnCl2	1.052e-10	1.052e-10	-9.978	-9.978	0.000	(0)	
MnCl3-	4.532e-14	3.926e-14	-13.344	-13.406	-0.062	(0)	
FeCl+2	1.735e-17	9.770e-18	-16.761	-17.010	-0.249	(0)	
FeCl2+	1.000e-19	8.667e-20	-19.000	-19.062	-0.062	(0)	
UO2Cl+	2.847e-21	2.377e-21	-20.546	-20.624	-0.078	(0)	
FeCl3	1.174e-23	1.174e-23	-22.930	-22.930	0.000	(0)	
UO2Cl2	1.931e-25	1.942e-25	-24.714	-24.712	0.002	(0)	
UCl+3	0.000e+00	0.000e+00	-40.673	-41.377	-0.705	(0)	
Fe(2)	3.801e-05						
Fe+2	2.940e-05	1.430e-05	-4.532	-4.845	-0.313	(0)	
FeSO4	7.952e-06	7.952e-06	-5.100	-5.100	0.000	(0)	
FeHCO3+	5.749e-07	5.008e-07	-6.240	-6.300	-0.060	(0)	
FeOH+	8.081e-08	7.001e-08	-7.093	-7.155	-0.062	(0)	
Fe(OH)2	5.989e-12	5.989e-12	-11.223	-11.223	0.000	(0)	
Fe(OH)3-	6.072e-13	5.260e-13	-12.217	-12.279	-0.062	(0)	
Fe(3)	1.040e-05						
Fe(OH)2+	9.797e-06	8.506e-06	-5.009	-5.070	-0.061	(0)	
Fe(OH)3	5.061e-07	5.061e-07	-6.296	-6.296	0.000	(0)	
Fe(OH)4-	9.479e-08	8.231e-08	-7.023	-7.085	-0.061	(0)	
FeOH+2	6.229e-11	3.508e-11	-10.206	-10.455	-0.249	(0)	
FeSO4+	7.744e-15	6.708e-15	-14.111	-14.173	-0.062	(0)	
Fe+3	1.319e-15	3.500e-16	-14.880	-15.456	-0.576	(0)	
Fe(SO4)2-	4.895e-16	4.088e-16	-15.310	-15.389	-0.078	(0)	
FeCl+2	1.735e-17	9.770e-18	-16.761	-17.010	-0.249	(0)	
Fe2(OH)2+4	1.123e-18	6.278e-20	-17.950	-19.202	-1.253	(0)	
FeCl2+	1.000e-19	8.667e-20	-19.000	-19.062	-0.062	(0)	

FeNO3+2	1.630e-20	7.928e-21	-19.788	-20.101	-0.313	(0)
FeHSeO3+2	1.669e-21	8.116e-22	-20.778	-21.091	-0.313	(0)
Fe3(OH)4+5	6.160e-22	6.800e-24	-21.210	-23.167	-1.957	(0)
FeCl3	1.174e-23	1.174e-23	-22.930	-22.930	0.000	(0)
H(0)	2.641e-21					
H2	1.320e-21	1.328e-21	-20.879	-20.877	0.002	(0)
K	1.058e-04					
K+	1.040e-04	8.974e-05	-3.983	-4.047	-0.064	(0)
KSO4-	1.769e-06	1.536e-06	-5.752	-5.814	-0.061	(0)
Mg	2.002e-03					
Mg+2	1.588e-03	8.807e-04	-2.799	-3.055	-0.256	(0)
MgSO4	3.767e-04	3.767e-04	-3.424	-3.424	0.000	(0)
MgHCO3+	3.474e-05	2.991e-05	-4.459	-4.524	-0.065	(0)
MgCO3	2.419e-06	2.419e-06	-5.616	-5.616	0.000	(0)
MgOH+	4.045e-08	3.533e-08	-7.393	-7.452	-0.059	(0)
MgUO2(CO3)3-2	1.538e-12	8.531e-13	-11.813	-12.069	-0.256	(0)
Mn(2)	8.164e-05					
Mn+2	6.627e-05	3.222e-05	-4.179	-4.492	-0.313	(0)
MnSO4	1.284e-05	1.284e-05	-4.892	-4.892	0.000	(0)
MnHCO3+	2.463e-06	2.134e-06	-5.608	-5.671	-0.062	(0)
MnCl+	6.345e-08	5.497e-08	-7.198	-7.260	-0.062	(0)
MnOH+	1.149e-08	9.957e-09	-7.940	-8.002	-0.062	(0)
MnCl2	1.052e-10	1.052e-10	-9.978	-9.978	0.000	(0)
MnNO3+	7.490e-11	6.255e-11	-10.126	-10.204	-0.078	(0)
MnCl3-	4.532e-14	3.926e-14	-13.344	-13.406	-0.062	(0)
Mn(NO3)2	1.978e-16	1.978e-16	-15.704	-15.704	0.000	(0)
Mn(OH)3-	1.738e-17	1.506e-17	-16.760	-16.822	-0.062	(0)
MnSe	1.809e-20	1.809e-20	-19.743	-19.743	0.000	(0)
Mn(OH)4-2	2.685e-23	1.512e-23	-22.571	-22.820	-0.249	(0)
MnSeO4	2.953e-24	2.953e-24	-23.530	-23.530	0.000	(0)
Mn(3)	2.270e-29					
Mn+3	2.270e-29	6.025e-30	-28.644	-29.220	-0.576	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-62.278	-62.528	-0.249	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-71.238	-71.305	-0.068	(0)
Mo	1.430e-07					
MoO4-2	1.429e-07	7.926e-08	-6.845	-7.101	-0.256	(0)
HMoO4-	4.383e-11	3.660e-11	-10.358	-10.437	-0.078	(0)
H2MoO4	1.864e-14	1.864e-14	-13.730	-13.730	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-52.172	-54.990	-2.818	(0)
HMo7O24-5	0.000e+00	0.000e+00	-54.208	-56.166	-1.957	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-57.642	-58.895	-1.253	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-62.420	-63.125	-0.705	(0)
N(-3)	1.544e-05					
NH4+	1.494e-05	1.273e-05	-4.826	-4.895	-0.069	(0)
NH4SO4-	4.076e-07	3.531e-07	-6.390	-6.452	-0.062	(0)
NH3	9.450e-08	9.450e-08	-7.025	-7.025	0.000	(0)
CaNH3+2	1.184e-09	5.757e-10	-8.927	-9.240	-0.313	(0)
Ca(NH3)2+2	1.057e-16	5.140e-17	-15.976	-16.289	-0.313	(0)
N(5)	1.430e-06					
NO3-	1.419e-06	1.225e-06	-5.848	-5.912	-0.064	(0)
CaNO3+	1.034e-08	8.636e-09	-7.985	-8.064	-0.078	(0)
MnNO3+	7.490e-11	6.255e-11	-10.126	-10.204	-0.078	(0)
Mn(NO3)2	1.978e-16	1.978e-16	-15.704	-15.704	0.000	(0)
FeNO3+2	1.630e-20	7.928e-21	-19.788	-20.101	-0.313	(0)
UO2NO3+	5.042e-24	4.211e-24	-23.297	-23.376	-0.078	(0)
Na	2.896e-03					
Na+	2.851e-03	2.460e-03	-2.545	-2.609	-0.064	(0)
NaSO4-	3.874e-05	3.363e-05	-4.412	-4.473	-0.061	(0)
NaHCO3	6.165e-06	6.165e-06	-5.210	-5.210	0.000	(0)
NaCO3-	2.983e-07	2.590e-07	-6.525	-6.587	-0.061	(0)
O(0)	8.760e-06					
O2	4.380e-06	4.405e-06	-5.359	-5.356	0.002	(0)
S(6)	6.180e-03					
SO4-2	4.668e-03	2.588e-03	-2.331	-2.587	-0.256	(0)

CaSO4	1.074e-03	1.074e-03	-2.969	-2.969	0.000	(0)
MgSO4	3.767e-04	3.767e-04	-3.424	-3.424	0.000	(0)
NaSO4-	3.874e-05	3.363e-05	-4.412	-4.473	-0.061	(0)
MnSO4	1.284e-05	1.284e-05	-4.892	-4.892	0.000	(0)
FeSO4	7.952e-06	7.952e-06	-5.100	-5.100	0.000	(0)
KSO4-	1.769e-06	1.536e-06	-5.752	-5.814	-0.061	(0)
NH4SO4-	4.076e-07	3.531e-07	-6.390	-6.452	-0.062	(0)
HSO4-	6.574e-09	5.678e-09	-8.182	-8.246	-0.064	(0)
FeSO4+	7.744e-15	6.708e-15	-14.111	-14.173	-0.062	(0)
Fe(SO4)2-	4.895e-16	4.088e-16	-15.310	-15.389	-0.078	(0)
UO2SO4	3.966e-18	3.966e-18	-17.402	-17.402	0.000	(0)
UO2(SO4)2-2	2.063e-19	1.003e-19	-18.685	-18.999	-0.313	(0)
U(SO4)2	5.421e-36	5.421e-36	-35.266	-35.266	0.000	(0)
USO4+2	8.216e-37	3.995e-37	-36.085	-36.398	-0.313	(0)
Se(-2)	5.298e-18					
HSe-	5.279e-18	4.408e-18	-17.277	-17.356	-0.078	(0)
MnSe	1.809e-20	1.809e-20	-19.743	-19.743	0.000	(0)
H2Se	1.048e-21	1.048e-21	-20.980	-20.980	0.000	(0)
Se-2	1.259e-25	6.122e-26	-24.900	-25.213	-0.313	(0)
Se(4)	1.902e-09					
HSeO3-	1.592e-09	1.330e-09	-8.798	-8.876	-0.078	(0)
SeO3-2	3.095e-10	1.505e-10	-9.509	-9.822	-0.313	(0)
H2SeO3	1.656e-14	1.656e-14	-13.781	-13.781	0.000	(0)
FeHSeO3+2	1.669e-21	8.116e-22	-20.778	-21.091	-0.313	(0)
Se(6)	7.778e-22					
SeO4-2	7.748e-22	4.297e-22	-21.111	-21.367	-0.256	(0)
MnSeO4	2.953e-24	2.953e-24	-23.530	-23.530	0.000	(0)
HSeO4-	5.693e-28	4.754e-28	-27.245	-27.323	-0.078	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-50.582	-51.287	-0.705	(0)
U(4)	1.665e-17					
U(OH)5-	1.663e-17	1.389e-17	-16.779	-16.857	-0.078	(0)
U(OH)4	2.290e-20	2.290e-20	-19.640	-19.640	0.000	(0)
U(OH)3+	3.759e-24	3.139e-24	-23.425	-23.503	-0.078	(0)
U(OH)2+2	1.360e-28	6.614e-29	-27.866	-28.180	-0.313	(0)
UOH+3	7.916e-34	1.563e-34	-33.101	-33.806	-0.705	(0)
U(SO4)2	5.421e-36	5.421e-36	-35.266	-35.266	0.000	(0)
USO4+2	8.216e-37	3.995e-37	-36.085	-36.398	-0.313	(0)
U+4	7.921e-40	0.000e+00	-39.101	-40.354	-1.253	(0)
UCl+3	0.000e+00	0.000e+00	-40.673	-41.377	-0.705	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-140.589	-146.930	-6.341	(0)
U(5)	5.159e-17					
UO2+	5.159e-17	4.308e-17	-16.287	-16.366	-0.078	(0)
U(6)	2.448e-09					
Ca2UO2(CO3)3	1.916e-09	1.927e-09	-8.718	-8.715	0.002	(0)
CaUO2(CO3)3-2	5.147e-10	2.854e-10	-9.288	-9.544	-0.256	(0)
UO2(CO3)3-4	1.281e-11	7.160e-13	-10.893	-12.145	-1.253	(0)
UO2(CO3)2-2	2.873e-12	1.397e-12	-11.542	-11.855	-0.313	(0)
MgUO2(CO3)3-2	1.538e-12	8.531e-13	-11.813	-12.069	-0.256	(0)
UO2(OH)2	6.491e-14	6.528e-14	-13.188	-13.185	0.002	(0)
UO2CO3	2.120e-14	2.120e-14	-13.674	-13.674	0.000	(0)
UO2(OH)3-	2.894e-15	2.497e-15	-14.539	-14.603	-0.064	(0)
UO2OH+	2.990e-17	2.497e-17	-16.524	-16.603	-0.078	(0)
UO2SO4	3.966e-18	3.966e-18	-17.402	-17.402	0.000	(0)
UO2+2	2.545e-18	1.412e-18	-17.594	-17.850	-0.256	(0)
UO2(SO4)2-2	2.063e-19	1.003e-19	-18.685	-18.999	-0.313	(0)
(UO2)2CO3(OH)3-	4.466e-20	3.854e-20	-19.350	-19.414	-0.064	(0)
UO2Cl+	2.847e-21	2.377e-21	-20.546	-20.624	-0.078	(0)
UO2(OH)4-2	2.168e-21	1.202e-21	-20.664	-20.920	-0.256	(0)
UO2NO3+	5.042e-24	4.211e-24	-23.297	-23.376	-0.078	(0)
UO2Cl2	1.931e-25	1.942e-25	-24.714	-24.712	0.002	(0)
(UO2)2(OH)2+2	5.203e-27	2.530e-27	-26.284	-26.597	-0.313	(0)
(UO2)3(CO3)6-6	8.568e-30	4.249e-32	-29.067	-31.372	-2.305	(0)
(UO2)2OH+3	4.552e-31	1.208e-31	-30.342	-30.918	-0.576	(0)
(UO2)3(OH)7-	7.784e-33	6.717e-33	-32.109	-32.173	-0.064	(0)
(UO2)3(OH)5+	4.088e-33	3.414e-33	-32.388	-32.467	-0.078	(0)

(UO2)3(OH)4+2 5.439e-36 3.016e-36 -35.264 -35.521 -0.256 (0)
 (UO2)4(OH)7+ 0.000e+00 0.000e+00 -40.859 -40.923 -0.064 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-31.61	-31.16	0.45 (NH4)2SeO4
Anhydrite	-0.97	-5.28	-4.31 CaSO4
Aragonite	0.13	-8.09	-8.21 CaCO3
Artinite	-6.99	3.47	10.47 MgCO3:Mg(OH)2:3H2O
Birnessite	-15.95	2.14	18.09 MnO2
Bixbyite	-13.75	-13.50	0.25 Mn2O3
Brucite	-5.74	11.92	17.67 Mg(OH)2
Calcite	0.34	-8.09	-8.42 CaCO3
CaMoO4	-1.86	-9.79	-7.94 CaMoO4
CaSeO3:2H2O	-7.03	-4.08	2.95 CaSeO3:2H2O
CaSeO4:2H2O	-21.10	-24.06	-2.96 CaSeO4:2H2O
CH4(g)	-48.59	-91.49	-42.90 CH4
CO2(g)	-2.20	-20.37	-18.18 CO2
Dolomite(disordered)	-0.33	-16.53	-16.21 CaMg(CO3)2
Dolomite(ordered)	0.27	-16.53	-16.80 CaMg(CO3)2
Epsomite	-3.43	-5.64	-2.21 MgSO4:7H2O
Fe(OH)2	-3.43	10.13	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	6.95	3.91	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-3.89	-2.34	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-14.44	-35.07	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-36.69	-38.67	-1.99 Fe2(SO4)3
Fe3(OH)8	3.94	24.16	20.22 Fe3(OH)8
FeMoO4	-1.93	-11.95	-10.01 FeMoO4
Ferrihydrite	3.29	7.01	3.72 Fe(OH)3
Ferroselite	-2.84	-21.78	-18.94 FeSe2
FeSe	-3.70	-14.71	-11.02 FeSe
Goethite	6.09	7.01	0.93 FeOOH
Gummite	-11.13	-2.87	8.26 UO3
Gypsum	-0.66	-5.28	-4.62 CaSO4:2H2O
H-Jarosite	-3.66	-14.09	-10.43 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-8.85	-22.08	-13.23 H2MoO4
H2Se(g)	-20.00	-24.85	-4.85 H2Se
Halite	-7.05	-5.48	1.58 NaCl
Hausmannite	-14.83	49.24	64.07 Mn3O4
Hematite	14.51	14.03	-0.49 Fe2O3
Huntite	-4.24	-33.43	-29.19 CaMg3(CO3)4
Hydromagnesite	-14.69	-21.87	-7.19 Mg5(CO3)4(OH)2:4H2O
K-Jarosite	3.21	-10.65	-13.86 KFe3(SO4)2(OH)6
K2MoO4	-18.48	-15.20	3.29 K2MoO4
K2SeO4	-28.73	-29.46	-0.73 K2SeO4
Lepidocrocite	5.64	7.01	1.37 FeOOH
Lime	-21.81	12.29	34.10 CaO
Maghemite	7.64	14.03	6.39 Fe2O3
Magnesioferrite	7.08	25.95	18.87 Fe2MgO4
Magnesite	-0.85	-8.45	-7.60 MgCO3
Magnetite	19.25	24.16	4.91 Fe3O4
Manganite	-5.96	19.38	25.34 MnOOH
Melanterite	-5.08	-7.43	-2.36 FeSO4:7H2O
Mg(OH)2(active)	-6.87	11.92	18.79 Mg(OH)2
MgMoO4	-8.31	-10.16	-1.85 MgMoO4
MgSeO3:6H2O	-7.46	-4.44	3.02 MgSeO3:6H2O
MgSeO4:6H2O	-23.22	-24.42	-1.20 MgSeO4:6H2O
Mirabilite	-6.12	-7.81	-1.69 Na2SO4:10H2O
Mn2(SO4)3	-61.67	-66.20	-4.53 Mn2(SO4)3
MnCl2:4H2O	-13.02	-10.23	2.79 MnCl2:4H2O
MnSe	-18.57	-14.36	4.21 MnSe
MnSeO3	-7.01	-5.88	1.13 MnSeO3
MnSeO3:2H2O	-6.80	-5.88	0.92 MnSeO3:2H2O
MnSeO4:5H2O	-23.81	-25.86	-2.05 MnSeO4:5H2O

MnSO4 -10.13 -7.08 3.05 MnSO4
MoO3 -14.08 -22.08 -8.00 MoO3
Na-Jarosite 0.90 -9.21 -10.11 NaFe3(SO4)2(OH)6
Na2Mo2O7 -17.40 -34.40 -17.00 Na2Mo2O7
Na2MoO4 -13.88 -12.32 1.56 Na2MoO4
Na2MoO4:2H2O -13.54 -12.32 1.22 Na2MoO4:2H2O
Na2SeO3:5H2O -16.91 -6.61 10.30 Na2SeO3:5H2O
Na2SeO4 -27.86 -26.58 1.28 Na2SeO4
Natron -8.83 -10.61 -1.79 Na2CO3:10H2O
Nesquehonite -3.96 -8.45 -4.50 MgCO3:3H2O
Nsutite -15.36 2.14 17.50 MnO2
O2(g) -51.66 35.56 87.22 O2
Periclase -10.75 11.92 22.68 MgO
Portlandite -11.44 12.29 23.73 Ca(OH)2
Pyrochroite -5.41 10.49 15.89 Mn(OH)2
Pyrolusite -15.08 28.27 43.34 MnO2
Rhodochrosite 0.68 -9.89 -10.57 MnCO3
Rutherfordine -8.77 -23.24 -14.48 UO2CO3
Schoepite -9.22 -2.87 6.35 UO2(OH)2:H2O
Semetal(am) 0.12 -7.07 -7.19 Se
Semetal(hex) 0.76 -7.07 -7.82 Se
SeO2 -16.48 -16.37 0.11 SeO2
SeO3 -58.45 -36.35 22.10 SeO3
Siderite -0.11 -10.24 -10.12 FeCO3
Thenardite -8.19 -7.81 0.39 Na2SO4
Thermonatrite -11.33 -10.61 0.71 Na2CO3:H2O
U3O8 -20.21 4.38 24.59 U3O8
U4O9 -23.86 -23.80 0.06 U4O9
UO2(am) -12.12 -10.39 1.73 UO2
UO2(NO3)2 -42.42 -29.67 12.75 UO2(NO3)2
UO2(NO3)2:2H2O -34.71 -29.67 5.03 UO2(NO3)2:2H2O
UO2(NO3)2:3H2O -33.13 -29.67 3.46 UO2(NO3)2:3H2O
UO2(NO3)2:6H2O -31.57 -29.68 1.90 UO2(NO3)2:6H2O
UO2(OH)2(beta) -8.89 -2.87 6.02 UO2(OH)2
UO2SeO4:4H2O -36.97 -39.22 -2.25 UO2SeO4:4H2O
UO3 -11.16 -2.87 8.28 UO3
Uraninite -6.29 -10.39 -4.11 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 11. 0943M

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

Elements	Molality	Moles
Alkalinity	6.824e-03	6.824e-03
Ca	5.023e-03	5.023e-03
Cl	4.266e-03	4.266e-03
Fe(2)	8.250e-05	8.250e-05
Fe(3)	1.076e-06	1.076e-06
K	2.136e-04	2.136e-04
Mg	2.575e-03	2.575e-03
Mn	5.287e-07	5.287e-07
Mo	8.247e-09	8.247e-09
N(-3)	3.575e-06	3.575e-06
N(5)	2.653e-04	2.653e-04
Na	7.493e-03	7.493e-03
O(0)	1.690e-05	1.690e-05
S(6)	6.287e-03	6.287e-03
Se	9.919e-08	9.919e-08
U	2.853e-08	2.853e-08

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

pH = 7.070
 pe = 1.400
 Activity of water = 0.999
 Ionic strength (mol/kgw) = 3.078e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 8.019e-03
 Total CO2 (mol/kg) = 8.019e-03
 Temperature (°C) = 15.40
 Electrical balance (eq) = -8.545e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -2.12
 Iterations = 21 (207 overall)
 Total H = 1.110229e+02
 Total O = 5.555685e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	2.2282	0.1276
N(-3)/N(5)	6.8532	0.3924
O(-2)/O(0)	13.8625	0.7936

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
H+	1.001e-07	8.511e-08	-7.000	-7.070	-0.070	0.00	
OH-	6.619e-08	5.591e-08	-7.179	-7.253	-0.073	(0)	
H2O	5.551e+01	9.994e-01	1.744	-0.000	0.000	18.03	
C(4)	8.019e-03						
HCO3-	6.518e-03	5.583e-03	-2.186	-2.253	-0.067	(0)	
H2CO3	1.209e-03	1.209e-03	-2.918	-2.918	0.000	(0)	
CaHCO3+	1.843e-04	1.585e-04	-3.735	-3.800	-0.066	(0)	
MgHCO3+	6.879e-05	5.833e-05	-4.162	-4.234	-0.072	(0)	
NaHCO3	2.368e-05	2.368e-05	-4.626	-4.626	0.000	(0)	
CaCO3	6.443e-06	6.443e-06	-5.191	-5.191	0.000	(0)	
CO3-2	4.830e-06	2.528e-06	-5.316	-5.597	-0.281	(0)	
FeHCO3+	1.936e-06	1.665e-06	-5.713	-5.779	-0.066	(0)	
MgCO3	1.928e-06	1.928e-06	-5.715	-5.715	0.000	(0)	
NaCO3-	4.529e-07	3.880e-07	-6.344	-6.411	-0.067	(0)	
MnHCO3+	2.359e-08	2.015e-08	-7.627	-7.696	-0.068	(0)	
Ca2UO2(CO3)3	2.187e-08	2.203e-08	-7.660	-7.657	0.003	(0)	
CaUO2(CO3)3-2	6.376e-09	3.337e-09	-8.195	-8.477	-0.281	(0)	
UO2(CO3)3-4	1.932e-10	7.532e-12	-9.714	-11.123	-1.409	(0)	
UO2(CO3)2-2	6.310e-11	2.804e-11	-10.200	-10.552	-0.352	(0)	
MgUO2(CO3)3-2	2.384e-11	1.248e-11	-10.623	-10.904	-0.281	(0)	
UO2CO3	6.530e-13	6.530e-13	-12.185	-12.185	0.000	(0)	
(UO2)2CO3(OH)3-	3.503e-18	2.979e-18	-17.456	-17.526	-0.070	(0)	
(UO2)3(CO3)6-6	7.550e-26	2.226e-28	-25.122	-27.653	-2.530	(0)	
Ca	5.023e-03						
Ca+2	3.808e-03	1.993e-03	-2.419	-2.700	-0.281	(0)	
CaSO4	1.022e-03	1.022e-03	-2.991	-2.991	0.000	(0)	
CaHCO3+	1.843e-04	1.585e-04	-3.735	-3.800	-0.066	(0)	
CaCO3	6.443e-06	6.443e-06	-5.191	-5.191	0.000	(0)	
CaNO3+	1.860e-06	1.519e-06	-5.731	-5.819	-0.088	(0)	
Ca2UO2(CO3)3	2.187e-08	2.203e-08	-7.660	-7.657	0.003	(0)	
CaUO2(CO3)3-2	6.376e-09	3.337e-09	-8.195	-8.477	-0.281	(0)	
CaOH+	2.313e-09	1.989e-09	-8.636	-8.701	-0.066	(0)	
CaNH3+2	1.101e-10	4.893e-11	-9.958	-10.310	-0.352	(0)	
Ca(NH3)2+2	8.548e-19	3.798e-19	-18.068	-18.420	-0.352	(0)	
Cl	4.266e-03						
Cl-	4.266e-03	3.628e-03	-2.370	-2.440	-0.070	(0)	
MnCl+	1.021e-09	8.719e-10	-8.991	-9.060	-0.068	(0)	
MnCl2	4.469e-12	4.469e-12	-11.350	-11.350	0.000	(0)	
MnCl3-	5.228e-15	4.466e-15	-14.282	-14.350	-0.068	(0)	

FeCl ₂	3.857e-17	2.054e-17	-16.414	-16.687	-0.274	(0)
FeCl ₂ ⁺	5.306e-19	4.532e-19	-18.275	-18.344	-0.068	(0)
UO ₂ Cl ⁺	3.980e-19	3.250e-19	-18.400	-18.488	-0.088	(0)
FeCl ₃	1.644e-22	1.644e-22	-21.784	-21.784	0.000	(0)
UO ₂ Cl ₂	6.706e-23	6.753e-23	-22.174	-22.170	0.003	(0)
UCl ₃	9.565e-38	1.542e-38	-37.019	-37.812	-0.793	(0)
Fe(2)	8.250e-05					
Fe ²⁺	6.485e-05	2.881e-05	-4.188	-4.540	-0.352	(0)
FeSO ₄	1.564e-05	1.564e-05	-4.806	-4.806	0.000	(0)
FeHCO ₃ ⁺	1.936e-06	1.665e-06	-5.713	-5.779	-0.066	(0)
FeOH ⁺	7.508e-08	6.413e-08	-7.124	-7.193	-0.068	(0)
Fe(OH) ₂	2.558e-12	2.558e-12	-11.592	-11.592	0.000	(0)
Fe(OH) ₃ ⁻	1.022e-13	8.729e-14	-12.991	-13.059	-0.068	(0)
Fe(3)	1.076e-06					
Fe(OH) ₂ ⁺	1.046e-06	8.962e-07	-5.980	-6.048	-0.067	(0)
Fe(OH) ₃	2.826e-08	2.826e-08	-7.549	-7.549	0.000	(0)
Fe(OH) ₄ ⁻	1.463e-09	1.253e-09	-8.835	-8.902	-0.067	(0)
FeOH ²⁺	2.088e-11	1.112e-11	-10.680	-10.954	-0.274	(0)
FeSO ₄ ⁺	5.900e-15	5.040e-15	-14.229	-14.298	-0.068	(0)
Fe ³⁺	1.095e-15	2.552e-16	-14.960	-15.593	-0.633	(0)
Fe(SO ₄) ₂ ⁻	3.512e-16	2.867e-16	-15.454	-15.543	-0.088	(0)
FeCl ₂	3.857e-17	2.054e-17	-16.414	-16.687	-0.274	(0)
FeNO ₃ ²⁺	2.114e-18	9.395e-19	-17.675	-18.027	-0.352	(0)
FeCl ₂ ⁺	5.306e-19	4.532e-19	-18.275	-18.344	-0.068	(0)
Fe ₂ (OH) ₂ ²⁺	1.488e-19	5.800e-21	-18.827	-20.237	-1.409	(0)
FeHSeO ₃ ²⁺	8.134e-20	3.614e-20	-19.090	-19.442	-0.352	(0)
FeCl ₃	1.644e-22	1.644e-22	-21.784	-21.784	0.000	(0)
Fe ₃ (OH) ₄ ⁵⁺	1.079e-23	6.784e-26	-22.967	-25.169	-2.202	(0)
H(0)	1.782e-20					
H ₂	8.909e-21	8.972e-21	-20.050	-20.047	0.003	(0)
K	2.136e-04					
K ⁺	2.102e-04	1.788e-04	-3.677	-3.748	-0.070	(0)
KSO ₄ ⁻	3.443e-06	2.949e-06	-5.463	-5.530	-0.067	(0)
Mg	2.575e-03					
Mg ²⁺	2.058e-03	1.077e-03	-2.686	-2.968	-0.281	(0)
MgSO ₄	4.465e-04	4.465e-04	-3.350	-3.350	0.000	(0)
MgHCO ₃ ⁺	6.879e-05	5.833e-05	-4.162	-4.234	-0.072	(0)
MgCO ₃	1.928e-06	1.928e-06	-5.715	-5.715	0.000	(0)
MgOH ⁺	2.366e-08	2.041e-08	-7.626	-7.690	-0.064	(0)
MgUO ₂ (CO ₃) ₃ ²⁻	2.384e-11	1.248e-11	-10.623	-10.904	-0.281	(0)
Mn(2)	5.287e-07					
Mn ²⁺	4.296e-07	1.909e-07	-6.367	-6.719	-0.352	(0)
MnSO ₄	7.436e-08	7.436e-08	-7.129	-7.129	0.000	(0)
MnHCO ₃ ⁺	2.359e-08	2.015e-08	-7.627	-7.696	-0.068	(0)
MnCl ⁺	1.021e-09	8.719e-10	-8.991	-9.060	-0.068	(0)
MnNO ₃ ⁺	8.303e-11	6.779e-11	-10.081	-10.169	-0.088	(0)
MnOH ⁺	3.138e-11	2.681e-11	-10.503	-10.572	-0.068	(0)
MnCl ₂	4.469e-12	4.469e-12	-11.350	-11.350	0.000	(0)
Mn(NO ₃) ₂	3.901e-14	3.901e-14	-13.409	-13.409	0.000	(0)
MnCl ₃ ⁻	5.228e-15	4.466e-15	-14.282	-14.350	-0.068	(0)
MnSe	7.609e-19	7.609e-19	-18.119	-18.119	0.000	(0)
Mn(OH) ₃ ⁻	5.735e-21	4.898e-21	-20.241	-20.310	-0.068	(0)
MnSeO ₄	1.079e-25	1.079e-25	-24.967	-24.967	0.000	(0)
Mn(OH) ₄ ²⁻	3.512e-27	1.870e-27	-26.454	-26.728	-0.274	(0)
Mn(3)	2.163e-31					
Mn ³⁺	2.163e-31	5.040e-32	-30.665	-31.298	-0.633	(0)
Mn(6)	0.000e+00					
MnO ₄ ²⁻	0.000e+00	0.000e+00	-66.853	-67.127	-0.274	(0)
Mn(7)	0.000e+00					
MnO ₄ ⁻	0.000e+00	0.000e+00	-75.674	-75.749	-0.075	(0)
Mo	8.247e-09					
MoO ₄ ²⁻	8.240e-09	4.313e-09	-8.084	-8.365	-0.281	(0)
HMoO ₄ ⁻	6.840e-12	5.585e-12	-11.165	-11.253	-0.088	(0)
H ₂ MoO ₄	6.455e-15	6.455e-15	-14.190	-14.190	0.000	(0)
Mo ₇ O ₂₄ ⁶⁻	0.000e+00	0.000e+00	-57.626	-60.797	-3.171	(0)
HMo ₇ O ₂₄ ⁵⁻	0.000e+00	0.000e+00	-59.336	-61.538	-2.202	(0)

H2Mo7O24-4 0.000e+00 0.000e+00 -62.434 -63.843 -1.409 (0)
 H3Mo7O24-3 0.000e+00 0.000e+00 -66.863 -67.656 -0.793 (0)
 N(-3) 3.575e-06
 NH4+ 3.476e-06 2.911e-06 -5.459 -5.536 -0.077 (0)
 NH4SO4- 8.989e-08 7.678e-08 -7.046 -7.115 -0.068 (0)
 NH3 9.703e-09 9.703e-09 -8.013 -8.013 0.000 (0)
 CaNH3+2 1.101e-10 4.893e-11 -9.958 -10.310 -0.352 (0)
 Ca(NH3)2+2 8.548e-19 3.798e-19 -18.068 -18.420 -0.352 (0)
 N(5) 2.653e-04
 NO3- 2.634e-04 2.241e-04 -3.579 -3.650 -0.070 (0)
 CaNO3+ 1.860e-06 1.519e-06 -5.731 -5.819 -0.088 (0)
 MnNO3+ 8.303e-11 6.779e-11 -10.081 -10.169 -0.088 (0)
 Mn(NO3)2 3.901e-14 3.901e-14 -13.409 -13.409 0.000 (0)
 FeNO3+2 2.114e-18 9.395e-19 -17.675 -18.027 -0.352 (0)
 UO2NO3+ 4.403e-20 3.595e-20 -19.356 -19.444 -0.088 (0)
 Na 7.493e-03
 Na+ 7.374e-03 6.272e-03 -2.132 -2.203 -0.070 (0)
 NaSO4- 9.551e-05 8.181e-05 -4.020 -4.087 -0.067 (0)
 NaHCO3 2.368e-05 2.368e-05 -4.626 -4.626 0.000 (0)
 NaCO3- 4.529e-07 3.880e-07 -6.344 -6.411 -0.067 (0)
 O(0) 1.690e-05
 O2 8.451e-06 8.511e-06 -5.073 -5.070 0.003 (0)
 S(6) 6.287e-03
 SO4-2 4.703e-03 2.462e-03 -2.328 -2.609 -0.281 (0)
 CaSO4 1.022e-03 1.022e-03 -2.991 -2.991 0.000 (0)
 MgSO4 4.465e-04 4.465e-04 -3.350 -3.350 0.000 (0)
 NaSO4- 9.551e-05 8.181e-05 -4.020 -4.087 -0.067 (0)
 FeSO4 1.564e-05 1.564e-05 -4.806 -4.806 0.000 (0)
 KSO4- 3.443e-06 2.949e-06 -5.463 -5.530 -0.067 (0)
 NH4SO4- 8.989e-08 7.678e-08 -7.046 -7.115 -0.068 (0)
 MnSO4 7.436e-08 7.436e-08 -7.129 -7.129 0.000 (0)
 HSO4- 1.791e-08 1.524e-08 -7.747 -7.817 -0.070 (0)
 FeSO4+ 5.900e-15 5.040e-15 -14.229 -14.298 -0.068 (0)
 Fe(SO4)2- 3.512e-16 2.867e-16 -15.454 -15.543 -0.088 (0)
 UO2SO4 1.950e-16 1.950e-16 -15.710 -15.710 0.000 (0)
 UO2(SO4)2-2 1.119e-17 4.971e-18 -16.951 -17.304 -0.352 (0)
 U(SO4)2 7.979e-33 7.979e-33 -32.098 -32.098 0.000 (0)
 USO4+2 1.284e-33 5.707e-34 -32.891 -33.244 -0.352 (0)
 Se(-2) 1.009e-13
 HSe- 1.008e-13 8.233e-14 -12.996 -13.084 -0.088 (0)
 H2Se 5.204e-17 5.204e-17 -16.284 -16.284 0.000 (0)
 MnSe 7.609e-19 7.609e-19 -18.119 -18.119 0.000 (0)
 Se-2 1.141e-21 5.071e-22 -20.943 -21.295 -0.352 (0)
 Se(4) 9.919e-08
 HSeO3- 9.181e-08 7.496e-08 -7.037 -7.125 -0.088 (0)
 SeO3-2 7.377e-09 3.278e-09 -8.132 -8.484 -0.352 (0)
 H2SeO3 2.504e-12 2.504e-12 -11.601 -11.601 0.000 (0)
 FeHSeO3+2 8.134e-20 3.614e-20 -19.090 -19.442 -0.352 (0)
 Se(6) 4.843e-21
 SeO4-2 4.842e-21 2.535e-21 -20.315 -20.596 -0.281 (0)
 MnSeO4 1.079e-25 1.079e-25 -24.967 -24.967 0.000 (0)
 HSeO4- 9.726e-27 7.941e-27 -26.012 -26.100 -0.088 (0)
 U(3) 0.000e+00
 U+3 0.000e+00 0.000e+00 -47.187 -47.979 -0.793 (0)
 U(4) 2.869e-16
 U(OH)5- 2.859e-16 2.334e-16 -15.544 -15.632 -0.088 (0)
 U(OH)4 9.750e-19 9.750e-19 -18.011 -18.011 0.000 (0)
 U(OH)3+ 4.187e-22 3.418e-22 -21.378 -21.466 -0.088 (0)
 U(OH)2+2 3.992e-26 1.774e-26 -25.399 -25.751 -0.352 (0)
 UOH+3 6.288e-31 1.014e-31 -30.201 -30.994 -0.793 (0)
 U(SO4)2 7.979e-33 7.979e-33 -32.098 -32.098 0.000 (0)
 USO4+2 1.284e-33 5.707e-34 -32.891 -33.244 -0.352 (0)
 U+4 1.663e-36 6.483e-38 -35.779 -37.188 -1.409 (0)
 UCl+3 9.565e-38 1.542e-38 -37.019 -37.812 -0.793 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -127.104 -134.238 -7.134 (0)
 U(5) 2.449e-15

UO2+ 2.449e-15 1.999e-15 -14.611 -14.699 -0.088 (0)
 U(6) 2.853e-08
 Ca2UO2(CO3)3 2.187e-08 2.203e-08 -7.660 -7.657 0.003 (0)
 CaUO2(CO3)3-2 6.376e-09 3.337e-09 -8.195 -8.477 -0.281 (0)
 UO2(CO3)3-4 1.932e-10 7.532e-12 -9.714 -11.123 -1.409 (0)
 UO2(CO3)2-2 6.310e-11 2.804e-11 -10.200 -10.552 -0.352 (0)
 MgUO2(CO3)3-2 2.384e-11 1.248e-11 -10.623 -10.904 -0.281 (0)
 UO2CO3 6.530e-13 6.530e-13 -12.185 -12.185 0.000 (0)
 UO2(OH)2 4.542e-13 4.574e-13 -12.343 -12.340 0.003 (0)
 UO2(OH)3- 7.820e-15 6.651e-15 -14.107 -14.177 -0.070 (0)
 UO2OH+ 6.570e-16 5.364e-16 -15.182 -15.270 -0.088 (0)
 UO2SO4 1.950e-16 1.950e-16 -15.710 -15.710 0.000 (0)
 UO2+2 1.308e-16 6.846e-17 -15.883 -16.165 -0.281 (0)
 UO2(SO4)2-2 1.119e-17 4.971e-18 -16.951 -17.304 -0.352 (0)
 (UO2)2CO3(OH)3- 3.503e-18 2.979e-18 -17.456 -17.526 -0.070 (0)
 UO2Cl+ 3.980e-19 3.250e-19 -18.400 -18.488 -0.088 (0)
 UO2NO3+ 4.403e-20 3.595e-20 -19.356 -19.444 -0.088 (0)
 UO2(OH)4-2 2.326e-21 1.217e-21 -20.633 -20.915 -0.281 (0)
 UO2Cl2 6.706e-23 6.753e-23 -22.174 -22.170 0.003 (0)
 (UO2)2(OH)2+2 2.213e-24 9.831e-25 -23.655 -24.007 -0.352 (0)
 (UO2)3(CO3)6-6 7.550e-26 2.226e-28 -25.122 -27.653 -2.530 (0)
 (UO2)2OH+3 4.635e-28 1.080e-28 -27.334 -27.967 -0.633 (0)
 (UO2)3(OH)5+ 5.350e-30 4.368e-30 -29.272 -29.360 -0.088 (0)
 (UO2)3(OH)7- 1.033e-30 8.785e-31 -29.986 -30.056 -0.070 (0)
 (UO2)3(OH)4+2 1.372e-32 7.183e-33 -31.863 -32.144 -0.281 (0)
 (UO2)4(OH)7+ 8.902e-38 7.571e-38 -37.051 -37.121 -0.070 (0)

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

Phase	SI**	log IAP	log K(288 K, 1 atm)
(NH4)2SeO4	-32.12	-31.67	0.45 (NH4)2SeO4
Anhydrite	-0.99	-5.31	-4.32 CaSO4
Aragonite	-0.07	-8.30	-8.23 CaCO3
Artinite	-7.69	2.61	10.30 MgCO3:Mg(OH)2:3H2O
Birnessite	-19.71	-1.62	18.09 MnO2
Bixbyite	-20.26	-20.18	0.08 Mn2O3
Brucite	-6.34	11.17	17.51 Mg(OH)2
Calcite	0.14	-8.30	-8.43 CaCO3
CaMoO4	-3.13	-11.07	-7.94 CaMoO4
CaSeO3:2H2O	-5.68	-2.76	2.93 CaSeO3:2H2O
CaSeO4:2H2O	-20.33	-23.30	-2.97 CaSeO4:2H2O
CH4(g)	-44.95	-87.50	-42.54 CH4
CO2(g)	-1.57	-19.74	-18.17 CO2
Dolomite(disordered)	-0.59	-16.86	-16.27 CaMg(CO3)2
Dolomite(ordered)	-0.00	-16.86	-16.86 CaMg(CO3)2
Epsomite	-3.38	-5.58	-2.19 MgSO4:7H2O
Fe(OH)2	-3.96	9.60	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	5.80	2.76	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-4.52	-2.96	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-10.73	-31.35	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-36.69	-39.01	-2.32 Fe2(SO4)3
Fe3(OH)8	0.61	20.83	20.22 Fe3(OH)8
FeMoO4	-2.88	-12.91	-10.03 FeMoO4
Ferrihydrite	2.00	5.62	3.62 Fe(OH)3
Ferroselite	5.10	-13.77	-18.87 FeSe2
FeSe	0.46	-10.55	-11.01 FeSe
Goethite	4.77	5.62	0.84 FeOOH
Gummitite	-10.17	-2.02	8.14 UO3
Gypsum	-0.69	-5.31	-4.62 CaSO4:2H2O
H-Jarosite	-5.89	-16.65	-10.76 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-9.34	-22.51	-13.16 H2MoO4
H2Se(g)	-15.28	-20.15	-4.87 H2Se
Halite	-6.22	-4.64	1.58 NaCl
Hausmannite	-24.28	39.20	63.48 Mn3O4
Hematite	11.90	11.23	-0.67 Fe2O3

Huntite	-4.65	-33.99	-29.34	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-15.60	-23.09	-7.49	Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O
K-Jarosite	0.71	-13.33	-14.04	KFe ₃ (SO ₄) ₂ (OH) ₆
K ₂ MoO ₄	-19.14	-15.86	3.28	K ₂ MoO ₄
K ₂ SeO ₄	-27.36	-28.09	-0.73	K ₂ SeO ₄
Lepidocrocite	4.25	5.62	1.37	FeOOH
Lime	-22.39	11.44	33.83	CaO
Maghemite	4.85	11.23	6.39	Fe ₂ O ₃
Magnesianoferrite	3.92	22.41	18.49	Fe ₂ MgO ₄
Magnesite	-0.99	-8.56	-7.58	MgCO ₃
Magnetite	16.21	20.83	4.62	Fe ₃ O ₄
Manganite	-9.45	15.89	25.34	MnOOH
Melanterite	-4.82	-7.15	-2.33	FeSO ₄ ·7H ₂ O
Mg(OH) ₂ (active)	-7.62	11.17	18.79	Mg(OH) ₂
MgMoO ₄	-9.48	-11.33	-1.85	MgMoO ₄
MgSeO ₃ ·6H ₂ O	-6.05	-3.02	3.02	MgSeO ₃ ·6H ₂ O
MgSeO ₄ ·6H ₂ O	-22.37	-23.57	-1.20	MgSeO ₄ ·6H ₂ O
Mirabilite	-5.44	-7.02	-1.58	Na ₂ SO ₄ ·10H ₂ O
Mn ₂ (SO ₄) ₃	-65.66	-70.42	-4.76	Mn ₂ (SO ₄) ₃
MnCl ₂ ·4H ₂ O	-14.38	-11.60	2.78	MnCl ₂ ·4H ₂ O
MnSe	-16.81	-12.73	4.07	MnSe
MnSeO ₃	-7.90	-6.77	1.13	MnSeO ₃
MnSeO ₃ ·2H ₂ O	-7.71	-6.77	0.93	MnSeO ₃ ·2H ₂ O
MnSeO ₄ ·5H ₂ O	-25.27	-27.32	-2.05	MnSeO ₄ ·5H ₂ O
MnSO ₄	-12.29	-9.33	2.96	MnSO ₄
MoO ₃	-14.50	-22.50	-8.00	MoO ₃
Na-Jarosite	-1.46	-11.78	-10.32	NaFe ₃ (SO ₄) ₂ (OH) ₆
Na ₂ Mo ₂ O ₇	-18.35	-35.28	-16.92	Na ₂ Mo ₂ O ₇
Na ₂ MoO ₄	-14.32	-12.77	1.55	Na ₂ MoO ₄
Na ₂ MoO ₄ ·2H ₂ O	-13.99	-12.77	1.22	Na ₂ MoO ₄ ·2H ₂ O
Na ₂ SeO ₃ ·5H ₂ O	-14.76	-4.46	10.30	Na ₂ SeO ₃ ·5H ₂ O
Na ₂ SeO ₄	-26.28	-25.00	1.28	Na ₂ SeO ₄
Natron	-8.31	-10.00	-1.69	Na ₂ CO ₃ ·10H ₂ O
Nesquehonite	-4.04	-8.57	-4.53	MgCO ₃ ·3H ₂ O
Nsutite	-19.12	-1.62	17.50	MnO ₂
O ₂ (g)	-52.54	33.88	86.42	O ₂
Periclase	-11.29	11.17	22.47	MgO
Portlandite	-12.11	11.44	23.55	Ca(OH) ₂
Pyrochroite	-8.34	7.42	15.76	Mn(OH) ₂
Pyrolusite	-18.61	24.36	42.97	MnO ₂
Rhodochrosite	-1.75	-12.32	-10.57	MnCO ₃
Rutherfordine	-7.28	-21.76	-14.48	UO ₂ CO ₃
Schoepite	-8.31	-2.03	6.28	UO ₂ (OH) ₂ ·H ₂ O
Semetal(am)	3.96	-3.21	-7.17	Se
Semetal(hex)	4.59	-3.21	-7.80	Se
SeO ₂	-14.31	-14.19	0.12	SeO ₂
SeO ₃	-56.63	-34.74	21.90	SeO ₃
Siderite	0.01	-10.14	-10.15	FeCO ₃
Thenardite	-7.39	-7.01	0.37	Na ₂ SO ₄
Thermonatrite	-10.70	-10.00	0.70	Na ₂ CO ₃ ·H ₂ O
U ₃ O ₈	-16.76	7.15	23.91	U ₃ O ₈
U ₄ O ₉	-18.16	-18.70	-0.53	U ₄ O ₉
UO ₂ (am)	-10.48	-8.91	1.57	UO ₂
UO ₂ (NO ₃) ₂	-36.10	-23.46	12.63	UO ₂ (NO ₃) ₂
UO ₂ (NO ₃) ₂ ·2H ₂ O	-28.46	-23.46	5.00	UO ₂ (NO ₃) ₂ ·2H ₂ O
UO ₂ (NO ₃) ₂ ·3H ₂ O	-26.91	-23.46	3.44	UO ₂ (NO ₃) ₂ ·3H ₂ O
UO ₂ (NO ₃) ₂ ·6H ₂ O	-25.39	-23.47	1.93	UO ₂ (NO ₃) ₂ ·6H ₂ O
UO ₂ (OH) ₂ (beta)	-7.97	-2.03	5.94	UO ₂ (OH) ₂
UO ₂ SeO ₄ ·4H ₂ O	-34.51	-36.76	-2.25	UO ₂ SeO ₄ ·4H ₂ O
UO ₃	-10.20	-2.02	8.17	UO ₃
Uraninite	-4.69	-8.91	-4.22	UO ₂

**For a gas, SI = log₁₀(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 12. 0951R

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

Elements	Molality	Moles
Alkalinity	6.343e-03	6.343e-03
Ca	4.623e-03	4.623e-03
Cl	3.983e-03	3.983e-03
Fe(2)	3.586e-07	3.586e-07
Fe(3)	7.173e-07	7.173e-07
K	2.131e-04	2.131e-04
Mg	2.497e-03	2.497e-03
Mn	9.114e-08	9.114e-08
Mo	1.889e-08	1.889e-08
N(-3)	3.575e-06	3.575e-06
N(5)	2.703e-04	2.703e-04
Na	7.275e-03	7.275e-03
O(0)	2.942e-05	2.942e-05
S(6)	5.796e-03	5.796e-03
Se	1.010e-07	1.010e-07
U	1.073e-07	1.073e-07

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

pH = 6.980
 pe = 4.300
 Activity of water = 0.999
 Ionic strength (mol/kgw) = 2.888e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 7.728e-03
 Total CO2 (mol/kg) = 7.728e-03
 Temperature (°C) = 15.20
 Electrical balance (eq) = -4.566e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -1.20
 Iterations = 13 (220 overall)
 Total H = 1.110228e+02
 Total O = 5.555404e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	4.5890	0.2625
N(-3)/N(5)	6.9789	0.3993
O(-2)/O(0)	14.0277	0.8025

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
H+	1.226e-07	1.047e-07	-6.911	-6.980	-0.069	0.00	
OH-	5.271e-08	4.472e-08	-7.278	-7.350	-0.071	(0)	
H2O	5.551e+01	9.995e-01	1.744	-0.000	0.000	18.03	
C(4)	7.728e-03						
HCO3-	6.076e-03	5.224e-03	-2.216	-2.282	-0.066	(0)	
H2CO3	1.395e-03	1.395e-03	-2.855	-2.855	0.000	(0)	
CaHCO3+	1.615e-04	1.394e-04	-3.792	-3.856	-0.064	(0)	
MgHCO3+	6.363e-05	5.418e-05	-4.196	-4.266	-0.070	(0)	
NaHCO3	2.170e-05	2.170e-05	-4.664	-4.664	0.000	(0)	
CaCO3	4.592e-06	4.592e-06	-5.338	-5.338	0.000	(0)	
CO3-2	3.600e-06	1.915e-06	-5.444	-5.718	-0.274	(0)	
MgCO3	1.446e-06	1.446e-06	-5.840	-5.840	0.000	(0)	
NaCO3-	3.354e-07	2.883e-07	-6.474	-6.540	-0.066	(0)	
Ca2UO2(CO3)3	8.141e-08	8.196e-08	-7.089	-7.086	0.003	(0)	
CaUO2(CO3)3-2	2.469e-08	1.313e-08	-7.607	-7.882	-0.274	(0)	

FeHCO3+	8.077e-09	6.971e-09	-8.093	-8.157	-0.064	(0)
MnHCO3+	3.911e-09	3.354e-09	-8.408	-8.474	-0.067	(0)
UO2(CO3)3-4	7.345e-10	3.172e-11	-9.134	-10.499	-1.365	(0)
UO2(CO3)2-2	3.365e-10	1.534e-10	-9.473	-9.814	-0.341	(0)
MgUO2(CO3)3-2	9.707e-11	5.162e-11	-10.013	-10.287	-0.274	(0)
UO2CO3	4.734e-12	4.734e-12	-11.325	-11.325	0.000	(0)
(UO2)2CO3(OH)3-	1.309e-16	1.118e-16	-15.883	-15.952	-0.069	(0)
(UO2)3(CO3)6-6	1.114e-23	3.791e-26	-22.953	-25.421	-2.468	(0)
Ca	4.623e-03					
Ca+2	3.543e-03	1.884e-03	-2.451	-2.725	-0.274	(0)
CaSO4	9.113e-04	9.113e-04	-3.040	-3.040	0.000	(0)
CaHCO3+	1.615e-04	1.394e-04	-3.792	-3.856	-0.064	(0)
CaCO3	4.592e-06	4.592e-06	-5.338	-5.338	0.000	(0)
CaNO3+	1.791e-06	1.471e-06	-5.747	-5.832	-0.085	(0)
Ca2UO2(CO3)3	8.141e-08	8.196e-08	-7.089	-7.086	0.003	(0)
CaUO2(CO3)3-2	2.469e-08	1.313e-08	-7.607	-7.882	-0.274	(0)
CaOH+	1.739e-09	1.501e-09	-8.760	-8.824	-0.064	(0)
CaNH3+2	8.304e-11	3.785e-11	-10.081	-10.422	-0.341	(0)
Ca(NH3)2+2	5.274e-19	2.404e-19	-18.278	-18.619	-0.341	(0)
Cl	3.983e-03					
Cl-	3.983e-03	3.401e-03	-2.400	-2.468	-0.069	(0)
MnCl+	1.697e-10	1.455e-10	-9.770	-9.837	-0.067	(0)
MnCl2	6.992e-13	6.992e-13	-12.155	-12.155	0.000	(0)
MnCl3-	7.638e-16	6.550e-16	-15.117	-15.184	-0.067	(0)
FeCl+2	3.603e-17	1.948e-17	-16.443	-16.710	-0.267	(0)
UO2Cl+	3.537e-18	2.906e-18	-17.451	-17.537	-0.085	(0)
FeCl2+	4.731e-19	4.057e-19	-18.325	-18.392	-0.067	(0)
UO2Cl2	5.650e-22	5.687e-22	-21.248	-21.245	0.003	(0)
FeCl3	1.380e-22	1.380e-22	-21.860	-21.860	0.000	(0)
UCl+3	0.000e+00	0.000e+00	-41.510	-42.278	-0.768	(0)
Fe(2)	3.586e-07					
Fe+2	2.840e-07	1.295e-07	-6.547	-6.888	-0.341	(0)
FeSO4	6.627e-08	6.627e-08	-7.179	-7.179	0.000	(0)
FeHCO3+	8.077e-09	6.971e-09	-8.093	-8.157	-0.064	(0)
FeOH+	2.688e-10	2.305e-10	-9.571	-9.637	-0.067	(0)
Fe(OH)2	7.337e-15	7.337e-15	-14.134	-14.134	0.000	(0)
Fe(OH)3-	2.369e-16	2.031e-16	-15.626	-15.692	-0.067	(0)
Fe(3)	7.173e-07					
Fe(OH)2+	7.016e-07	6.032e-07	-6.154	-6.220	-0.066	(0)
Fe(OH)3	1.500e-08	1.500e-08	-7.824	-7.824	0.000	(0)
Fe(OH)4-	6.481e-10	5.572e-10	-9.188	-9.254	-0.066	(0)
FeOH+2	1.682e-11	9.094e-12	-10.774	-11.041	-0.267	(0)
FeSO4+	5.618e-15	4.818e-15	-14.250	-14.317	-0.067	(0)
Fe+3	1.076e-15	2.600e-16	-14.968	-15.585	-0.617	(0)
Fe(SO4)2-	3.158e-16	2.595e-16	-15.501	-15.586	-0.085	(0)
FeCl+2	3.603e-17	1.948e-17	-16.443	-16.710	-0.267	(0)
FeNO3+2	2.171e-18	9.899e-19	-17.663	-18.004	-0.341	(0)
FeCl2+	4.731e-19	4.057e-19	-18.325	-18.392	-0.067	(0)
Fe2(OH)2+4	9.058e-20	3.912e-21	-19.043	-20.408	-1.365	(0)
FeHSeO3+2	8.340e-20	3.802e-20	-19.079	-19.420	-0.341	(0)
FeCl3	1.380e-22	1.380e-22	-21.860	-21.860	0.000	(0)
Fe3(OH)4+5	4.166e-24	3.072e-26	-23.380	-25.513	-2.132	(0)
H(0)	4.285e-26					
H2	2.143e-26	2.157e-26	-25.669	-25.666	0.003	(0)
K	2.131e-04					
K+	2.099e-04	1.792e-04	-3.678	-3.747	-0.069	(0)
KSO4-	3.246e-06	2.791e-06	-5.489	-5.554	-0.066	(0)
Mg	2.497e-03					
Mg+2	2.013e-03	1.071e-03	-2.696	-2.970	-0.274	(0)
MgSO4	4.187e-04	4.187e-04	-3.378	-3.378	0.000	(0)
MgHCO3+	6.363e-05	5.418e-05	-4.196	-4.266	-0.070	(0)
MgCO3	1.446e-06	1.446e-06	-5.840	-5.840	0.000	(0)
MgOH+	1.868e-08	1.617e-08	-7.729	-7.791	-0.063	(0)
MgUO2(CO3)3-2	9.707e-11	5.162e-11	-10.013	-10.287	-0.274	(0)
Mn(2)	9.114e-08					
Mn+2	7.456e-08	3.399e-08	-7.127	-7.469	-0.341	(0)

MnSO4	1.248e-08	1.248e-08	-7.904	-7.904	0.000	(0)
MnHCO3+	3.911e-09	3.354e-09	-8.408	-8.474	-0.067	(0)
MnCl+	1.697e-10	1.455e-10	-9.770	-9.837	-0.067	(0)
MnNO3+	1.503e-11	1.235e-11	-10.823	-10.908	-0.085	(0)
MnOH+	4.452e-12	3.818e-12	-11.351	-11.418	-0.067	(0)
MnCl2	6.992e-13	6.992e-13	-12.155	-12.155	0.000	(0)
Mn(NO3)2	7.276e-15	7.276e-15	-14.138	-14.138	0.000	(0)
MnCl3-	7.638e-16	6.550e-16	-15.117	-15.184	-0.067	(0)
MnSeO4	6.364e-21	6.364e-21	-20.196	-20.196	0.000	(0)
Mn(OH)3-	5.463e-22	4.684e-22	-21.263	-21.329	-0.067	(0)
Mn(OH)4-2	2.688e-28	1.454e-28	-27.571	-27.838	-0.267	(0)
MnSe	1.581e-36	1.581e-36	-35.801	-35.801	0.000	(0)
Mn(3)	2.861e-29					
Mn+3	2.861e-29	6.910e-30	-28.544	-29.161	-0.617	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-56.818	-57.085	-0.267	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-62.749	-62.822	-0.073	(0)
Mo	1.889e-08					
MoO4-2	1.887e-08	1.004e-08	-7.724	-7.998	-0.274	(0)
HMoO4-	1.935e-11	1.590e-11	-10.713	-10.799	-0.085	(0)
H2MoO4	2.291e-14	2.291e-14	-13.640	-13.640	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-54.410	-57.480	-3.070	(0)
HMo7O24-5	0.000e+00	0.000e+00	-56.001	-58.133	-2.132	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-58.984	-60.348	-1.365	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-63.303	-64.071	-0.768	(0)
N(-3)	3.575e-06					
NH4+	3.482e-06	2.930e-06	-5.458	-5.533	-0.075	(0)
NH4SO4-	8.519e-08	7.306e-08	-7.070	-7.136	-0.067	(0)
NH3	7.822e-09	7.822e-09	-8.107	-8.107	0.000	(0)
CaNH3+2	8.304e-11	3.785e-11	-10.081	-10.422	-0.341	(0)
Ca(NH3)2+2	5.274e-19	2.404e-19	-18.278	-18.619	-0.341	(0)
N(5)	2.703e-04					
NO3-	2.685e-04	2.293e-04	-3.571	-3.640	-0.069	(0)
CaNO3+	1.791e-06	1.471e-06	-5.747	-5.832	-0.085	(0)
MnNO3+	1.503e-11	1.235e-11	-10.823	-10.908	-0.085	(0)
Mn(NO3)2	7.276e-15	7.276e-15	-14.138	-14.138	0.000	(0)
FeNO3+2	2.171e-18	9.899e-19	-17.663	-18.004	-0.341	(0)
UO2NO3+	4.305e-19	3.538e-19	-18.366	-18.451	-0.085	(0)
Na	7.275e-03					
Na+	7.165e-03	6.119e-03	-2.145	-2.213	-0.069	(0)
NaSO4-	8.771e-05	7.541e-05	-4.057	-4.123	-0.066	(0)
NaHCO3	2.170e-05	2.170e-05	-4.664	-4.664	0.000	(0)
NaCO3-	3.354e-07	2.883e-07	-6.474	-6.540	-0.066	(0)
O(0)	2.942e-05					
O2	1.471e-05	1.481e-05	-4.832	-4.830	0.003	(0)
S(6)	5.796e-03					
SO4-2	4.375e-03	2.327e-03	-2.359	-2.633	-0.274	(0)
CaSO4	9.113e-04	9.113e-04	-3.040	-3.040	0.000	(0)
MgSO4	4.187e-04	4.187e-04	-3.378	-3.378	0.000	(0)
NaSO4-	8.771e-05	7.541e-05	-4.057	-4.123	-0.066	(0)
KSO4-	3.246e-06	2.791e-06	-5.489	-5.554	-0.066	(0)
NH4SO4-	8.519e-08	7.306e-08	-7.070	-7.136	-0.067	(0)
FeSO4	6.627e-08	6.627e-08	-7.179	-7.179	0.000	(0)
HSO4-	2.061e-08	1.761e-08	-7.686	-7.754	-0.068	(0)
MnSO4	1.248e-08	1.248e-08	-7.904	-7.904	0.000	(0)
FeSO4+	5.618e-15	4.818e-15	-14.250	-14.317	-0.067	(0)
UO2SO4	1.756e-15	1.756e-15	-14.755	-14.755	0.000	(0)
Fe(SO4)2-	3.158e-16	2.595e-16	-15.501	-15.586	-0.085	(0)
UO2(SO4)2-2	9.233e-17	4.209e-17	-16.035	-16.376	-0.341	(0)
U(SO4)2	2.561e-37	2.561e-37	-36.592	-36.592	0.000	(0)
USO4+2	4.282e-38	1.952e-38	-37.368	-37.710	-0.341	(0)
Se(-2)	1.439e-30					
HSe-	1.438e-30	1.182e-30	-29.842	-29.927	-0.085	(0)
H2Se	9.182e-34	9.182e-34	-33.037	-33.037	0.000	(0)
MnSe	1.581e-36	1.581e-36	-35.801	-35.801	0.000	(0)

Se-2 1.280e-38 5.836e-39 -37.893 -38.234 -0.341 (0)
 Se(4) 1.010e-07
 HSeO3- 9.488e-08 7.796e-08 -7.023 -7.108 -0.085 (0)
 SeO3-2 6.070e-09 2.767e-09 -8.217 -8.558 -0.341 (0)
 H2SeO3 3.199e-12 3.199e-12 -11.495 -11.495 0.000 (0)
 FeHSeO3+2 8.340e-20 3.802e-20 -19.079 -19.420 -0.341 (0)
 Se(6) 1.585e-15
 SeO4-2 1.585e-15 8.428e-16 -14.800 -15.074 -0.274 (0)
 MnSeO4 6.364e-21 6.364e-21 -20.196 -20.196 0.000 (0)
 HSeO4- 3.927e-21 3.227e-21 -20.406 -20.491 -0.085 (0)
 U(3) 0.000e+00
 U+3 0.000e+00 0.000e+00 -54.565 -55.333 -0.768 (0)
 U(4) 3.551e-21
 U(OH)5- 3.536e-21 2.906e-21 -20.451 -20.537 -0.085 (0)
 U(OH)4 1.498e-23 1.498e-23 -22.824 -22.824 0.000 (0)
 U(OH)3+ 7.886e-27 6.480e-27 -26.103 -26.188 -0.085 (0)
 U(OH)2+2 9.128e-31 4.161e-31 -30.040 -30.381 -0.341 (0)
 UOH+3 1.726e-35 2.948e-36 -34.763 -35.531 -0.768 (0)
 U(SO4)2 2.561e-37 2.561e-37 -36.592 -36.592 0.000 (0)
 USO4+2 4.282e-38 1.952e-38 -37.368 -37.710 -0.341 (0)
 U+4 0.000e+00 0.000e+00 -40.264 -41.629 -1.365 (0)
 UCl+3 0.000e+00 0.000e+00 -41.510 -42.278 -0.768 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -155.322 -162.230 -6.909 (0)
 U(5) 2.947e-17
 UO2+ 2.947e-17 2.422e-17 -16.531 -16.616 -0.085 (0)
 U(6) 1.073e-07
 Ca2UO2(CO3)3 8.141e-08 8.196e-08 -7.089 -7.086 0.003 (0)
 CaUO2(CO3)3-2 2.469e-08 1.313e-08 -7.607 -7.882 -0.274 (0)
 UO2(CO3)3-4 7.345e-10 3.172e-11 -9.134 -10.499 -1.365 (0)
 UO2(CO3)2-2 3.365e-10 1.534e-10 -9.473 -9.814 -0.341 (0)
 MgUO2(CO3)3-2 9.707e-11 5.162e-11 -10.013 -10.287 -0.274 (0)
 UO2CO3 4.734e-12 4.734e-12 -11.325 -11.325 0.000 (0)
 UO2(OH)2 2.877e-12 2.896e-12 -11.541 -11.538 0.003 (0)
 UO2(OH)3- 4.009e-14 3.423e-14 -13.397 -13.466 -0.069 (0)
 UO2OH+ 5.016e-15 4.121e-15 -14.300 -14.385 -0.085 (0)
 UO2SO4 1.756e-15 1.756e-15 -14.755 -14.755 0.000 (0)
 UO2+2 1.233e-15 6.560e-16 -14.909 -15.183 -0.274 (0)
 (UO2)2CO3(OH)3- 1.309e-16 1.118e-16 -15.883 -15.952 -0.069 (0)
 UO2(SO4)2-2 9.233e-17 4.209e-17 -16.035 -16.376 -0.341 (0)
 UO2Cl+ 3.537e-18 2.906e-18 -17.451 -17.537 -0.085 (0)
 UO2NO3+ 4.305e-19 3.538e-19 -18.366 -18.451 -0.085 (0)
 UO2(OH)4-2 9.575e-21 5.092e-21 -20.019 -20.293 -0.274 (0)
 UO2Cl2 5.650e-22 5.687e-22 -21.248 -21.245 0.003 (0)
 (UO2)2(OH)2+2 1.293e-22 5.894e-23 -21.888 -22.230 -0.341 (0)
 (UO2)3(CO3)6-6 1.114e-23 3.791e-26 -22.953 -25.421 -2.468 (0)
 (UO2)2OH+3 3.337e-26 8.062e-27 -25.477 -26.094 -0.617 (0)
 (UO2)3(OH)5+ 1.609e-27 1.322e-27 -26.793 -26.879 -0.085 (0)
 (UO2)3(OH)7- 2.123e-28 1.813e-28 -27.673 -27.742 -0.069 (0)
 (UO2)3(OH)4+2 5.189e-30 2.760e-30 -29.285 -29.559 -0.274 (0)
 (UO2)4(OH)7+ 1.753e-34 1.497e-34 -33.756 -33.825 -0.069 (0)

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

Phase SI** log IAP log K(288 K, 1 atm)

(NH4)2SeO4 -26.59 -26.14 0.45 (NH4)2SeO4
 Anhydrite -1.04 -5.36 -4.32 CaSO4
 Aragonite -0.21 -8.44 -8.23 CaCO3
 Artinite -8.02 2.30 10.32 MgCO3:Mg(OH)2:3H2O
 Birnessite -15.03 3.06 18.09 MnO2
 Bixbyite -16.54 -16.44 0.10 Mn2O3
 Brucite -6.53 10.99 17.52 Mg(OH)2
 Calcite -0.01 -8.44 -8.43 CaCO3
 CaMoO4 -2.79 -10.72 -7.94 CaMoO4
 CaSeO3:2H2O -5.78 -2.85 2.93 CaSeO3:2H2O
 CaSeO4:2H2O -14.83 -17.80 -2.97 CaSeO4:2H2O

CH4(g) -67.34 -109.92 -42.58 CH4
 CO2(g) -1.51 -19.68 -18.17 CO2
 Dolomite(disordered) -0.87 -17.13 -16.26 CaMg(CO3)2
 Dolomite(ordered) -0.28 -17.13 -16.85 CaMg(CO3)2
 Epsomite -3.41 -5.61 -2.20 MgSO4:7H2O
 Fe(OH)2 -6.49 7.07 13.56 Fe(OH)2
 Fe(OH)2.7Cl.3 5.56 2.52 -3.04 Fe(OH)2.7Cl.3
 Fe2(OH)4SeO3 -4.93 -3.38 1.55 Fe2(OH)4SeO3
 Fe2(SeO3)3:2H2O -10.93 -31.55 -20.63 Fe2(SeO3)3:2H2O
 Fe2(SO4)3 -36.78 -39.07 -2.29 Fe2(SO4)3
 Fe3(OH)8 -2.44 17.78 20.22 Fe3(OH)8
 FeMoO4 -4.86 -14.89 -10.02 FeMoO4
 Ferrihydrite 1.73 5.35 3.63 Fe(OH)3
 Ferroselite -25.31 -44.18 -18.88 FeSe2
 FeSe -18.82 -29.84 -11.01 FeSe
 Goethite 4.50 5.35 0.85 FeOOH
 Gummite -9.38 -1.22 8.15 UO3
 Gypsum -0.74 -5.36 -4.62 CaSO4:2H2O
 H-Jarosite -6.40 -17.12 -10.73 (H3O)Fe3(SO4)2(OH)6
 H2MoO4 -8.79 -21.96 -13.17 H2MoO4
 H2Se(g) -32.04 -36.91 -4.87 H2Se
 Halite -6.26 -4.68 1.58 NaCl
 Hausmannite -21.50 42.03 63.54 Mn3O4
 Hematite 11.36 10.71 -0.65 Fe2O3
 Huntite -5.18 -34.51 -29.33 CaMg3(CO3)4
 Hydromagnesite -16.30 -23.76 -7.47 Mg5(CO3)4(OH)2:4H2O
 K-Jarosite 0.13 -13.89 -14.02 KFe3(SO4)2(OH)6
 K2MoO4 -18.77 -15.49 3.28 K2MoO4
 K2SeO4 -21.84 -22.57 -0.73 K2SeO4
 Lepidocrocite 3.98 5.35 1.37 FeOOH
 Lime -22.62 11.23 33.85 CaO
 Maghemite 4.32 10.71 6.39 Fe2O3
 Magnesioferrite 3.18 21.70 18.52 Fe2MgO4
 Magnesite -1.11 -8.69 -7.58 MgCO3
 Magnetite 13.14 17.78 4.64 Fe3O4
 Manganite -7.57 17.77 25.34 MnOOH
 Melanterite -7.19 -9.52 -2.33 FeSO4:7H2O
 Mg(OH)2(active) -7.80 10.99 18.79 Mg(OH)2
 MgMoO4 -9.12 -10.97 -1.85 MgMoO4
 MgSeO3:6H2O -6.12 -3.10 3.02 MgSeO3:6H2O
 MgSeO4:6H2O -16.85 -18.05 -1.20 MgSeO4:6H2O
 Mirabilite -5.48 -7.06 -1.59 Na2SO4:10H2O
 Mn2(SO4)3 -61.48 -66.22 -4.74 Mn2(SO4)3
 MnCl2:4H2O -15.19 -12.41 2.78 MnCl2:4H2O
 MnSe -34.50 -30.42 4.08 MnSe
 MnSeO3 -8.73 -7.60 1.13 MnSeO3
 MnSeO3:2H2O -8.53 -7.60 0.93 MnSeO3:2H2O
 MnSeO4:5H2O -20.49 -22.54 -2.05 MnSeO4:5H2O
 MnSO4 -13.07 -10.10 2.97 MnSO4
 MoO3 -13.96 -21.96 -8.00 MoO3
 Na-Jarosite -2.06 -12.36 -10.30 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -17.45 -34.38 -16.93 Na2Mo2O7
 Na2MoO4 -13.97 -12.43 1.55 Na2MoO4
 Na2MoO4:2H2O -13.65 -12.43 1.22 Na2MoO4:2H2O
 Na2SeO3:5H2O -14.86 -4.56 10.30 Na2SeO3:5H2O
 Na2SeO4 -20.78 -19.50 1.28 Na2SeO4
 Natron -8.44 -10.15 -1.70 Na2CO3:10H2O
 Nesquehonite -4.16 -8.69 -4.53 MgCO3:3H2O
 Nsutite -14.44 3.06 17.50 MnO2
 O2(g) -41.37 45.12 86.49 O2
 Periclase -11.50 10.99 22.48 MgO
 Portlandite -12.34 11.23 23.57 Ca(OH)2
 Pyrochroite -9.28 6.49 15.77 Mn(OH)2
 Pyrolusite -13.95 29.05 43.00 MnO2
 Rhodochrosite -2.62 -13.19 -10.57 MnCO3
 Rutherfordine -6.42 -20.90 -14.48 UO2CO3

Schoepite -7.51 -1.22 6.29 UO₂(OH)₂:H₂O
 Semetal(am) -7.17 -14.35 -7.17 Se
 Semetal(hex) -6.54 -14.35 -7.80 Se
 SeO₂ -14.20 -14.09 0.12 SeO₂
 SeO₃ -50.95 -29.03 21.92 SeO₃
 Siderite -2.46 -12.61 -10.14 FeCO₃
 Thenardite -7.44 -7.06 0.38 Na₂SO₄
 Thermonatrite -10.84 -10.14 0.70 Na₂CO₃:H₂O
 U₃O₈ -19.98 3.99 23.97 U₃O₈
 U₄O₉ -31.80 -32.28 -0.48 U₄O₉
 UO₂(am) -15.30 -13.71 1.59 UO₂
 UO₂(NO₃)₂ -35.11 -22.46 12.64 UO₂(NO₃)₂
 UO₂(NO₃)₂:2H₂O -27.46 -22.46 5.00 UO₂(NO₃)₂:2H₂O
 UO₂(NO₃)₂:3H₂O -25.91 -22.46 3.44 UO₂(NO₃)₂:3H₂O
 UO₂(NO₃)₂:6H₂O -24.39 -22.46 1.92 UO₂(NO₃)₂:6H₂O
 UO₂(OH)₂(beta) -7.17 -1.22 5.95 UO₂(OH)₂
 UO₂SeO₄:4H₂O -28.01 -30.26 -2.25 UO₂SeO₄:4H₂O
 UO₃ -9.41 -1.22 8.18 UO₃
 Uraninite -9.50 -13.71 -4.21 UO₂

**For a gas, SI = log₁₀(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 13. SAG1-1

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

Elements	Molality	Moles
Alkalinity	4.181e-03	4.181e-03
Ca	3.272e-03	3.272e-03
Cl	2.033e-03	2.033e-03
Fe(2)	8.604e-05	8.604e-05
Fe(3)	1.434e-04	1.434e-04
K	1.034e-04	1.034e-04
Mg	1.882e-03	1.882e-03
Mn	1.345e-05	1.345e-05
Mo	2.859e-07	2.859e-07
N(-3)	2.008e-05	2.008e-05
N(5)	1.429e-06	1.429e-06
Na	4.271e-03	4.271e-03
O(0)	1.251e-05	1.251e-05
S(6)	4.647e-03	4.647e-03
Se	1.521e-09	1.521e-09
U	5.047e-09	5.047e-09

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

pH = 7.570
 pe = 0.500
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.098e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 4.389e-03
 Total CO₂ (mol/kg) = 4.389e-03
 Temperature (°C) = 14.20
 Electrical balance (eq) = -4.646e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -1.77
 Iterations = 12 (232 overall)
 Total H = 1.110187e+02
 Total O = 5.553891e+01

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

Redox couple	pe Eh (volts)
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Fe(2)/Fe(3)	3.2851	0.1873
N(-3)/N(5)	5.9248	0.3378
O(-2)/O(0)	13.4204	0.7651

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

Species	Log Molality	Log Activity	Log Molality	Log Activity	Log mole V	Gamma	cm ³ /mol
OH-	1.852e-07	1.605e-07	-6.732	-6.795	-0.062	(0)	
H+	3.092e-08	2.692e-08	-7.510	-7.570	-0.060	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	
C(4)	4.389e-03						
HCO3-	3.999e-03	3.501e-03	-2.398	-2.456	-0.058	(0)	
H2CO3	2.435e-04	2.435e-04	-3.613	-3.613	0.000	(0)	
CaHCO3+	8.035e-05	7.054e-05	-4.095	-4.152	-0.057	(0)	
MgHCO3+	3.425e-05	2.976e-05	-4.465	-4.526	-0.061	(0)	
CaCO3	8.906e-06	8.906e-06	-5.050	-5.050	0.000	(0)	
NaHCO3	8.897e-06	8.897e-06	-5.051	-5.051	0.000	(0)	
CO3-2	8.512e-06	4.887e-06	-5.070	-5.311	-0.241	(0)	
MgCO3	2.991e-06	2.991e-06	-5.524	-5.524	0.000	(0)	
FeHCO3+	1.411e-06	1.239e-06	-5.851	-5.907	-0.057	(0)	
NaCO3-	5.194e-07	4.547e-07	-6.285	-6.342	-0.058	(0)	
MnHCO3+	4.296e-07	3.753e-07	-6.367	-6.426	-0.059	(0)	
Ca2UO2(CO3)3	3.672e-09	3.689e-09	-8.435	-8.433	0.002	(0)	
CaUO2(CO3)3-2	1.324e-09	7.604e-10	-8.878	-9.119	-0.241	(0)	
UO2(CO3)3-4	3.627e-11	2.503e-12	-10.440	-11.602	-1.161	(0)	
UO2(CO3)2-2	8.530e-12	4.372e-12	-11.069	-11.359	-0.290	(0)	
MgUO2(CO3)3-2	5.518e-12	3.168e-12	-11.258	-11.499	-0.241	(0)	
UO2CO3	5.378e-14	5.378e-14	-13.269	-13.269	0.000	(0)	
(UO2)2CO3(OH)3-	3.952e-19	3.440e-19	-18.403	-18.463	-0.060	(0)	
(UO2)3(CO3)6-6	1.575e-28	1.068e-30	-27.803	-29.971	-2.169	(0)	
Ca	3.272e-03						
Ca+2	2.552e-03	1.465e-03	-2.593	-2.834	-0.241	(0)	
CaSO4	6.306e-04	6.306e-04	-3.200	-3.200	0.000	(0)	
CaHCO3+	8.035e-05	7.054e-05	-4.095	-4.152	-0.057	(0)	
CaCO3	8.906e-06	8.906e-06	-5.050	-5.050	0.000	(0)	
CaNO3+	7.358e-09	6.225e-09	-8.133	-8.206	-0.073	(0)	
CaOH+	4.712e-09	4.137e-09	-8.327	-8.383	-0.057	(0)	
Ca2UO2(CO3)3	3.672e-09	3.689e-09	-8.435	-8.433	0.002	(0)	
CaUO2(CO3)3-2	1.324e-09	7.604e-10	-8.878	-9.119	-0.241	(0)	
CaNH3+2	1.280e-09	6.559e-10	-8.893	-9.183	-0.290	(0)	
Ca(NH3)2+2	1.811e-16	9.284e-17	-15.742	-16.032	-0.290	(0)	
Cl	2.033e-03						
Cl-	2.033e-03	1.770e-03	-2.692	-2.752	-0.060	(0)	
MnCl+	1.456e-08	1.272e-08	-7.837	-7.896	-0.059	(0)	
MnCl2	3.179e-11	3.179e-11	-10.498	-10.498	0.000	(0)	
MnCl3-	1.774e-14	1.550e-14	-13.751	-13.810	-0.059	(0)	
FeCl+2	2.128e-16	1.240e-16	-15.672	-15.907	-0.235	(0)	
FeCl2+	1.590e-18	1.389e-18	-17.799	-17.857	-0.059	(0)	
UO2Cl+	7.816e-21	6.613e-21	-20.107	-20.180	-0.073	(0)	
FeCl3	2.457e-22	2.457e-22	-21.610	-21.610	0.000	(0)	
UO2Cl2	6.859e-25	6.892e-25	-24.164	-24.162	0.002	(0)	
UCl+3	1.218e-39	2.707e-40	-38.914	-39.567	-0.653	(0)	
Fe(2)	8.604e-05						
Fe+2	6.842e-05	3.507e-05	-4.165	-4.455	-0.290	(0)	
FeSO4	1.595e-05	1.595e-05	-4.797	-4.797	0.000	(0)	
FeHCO3+	1.411e-06	1.239e-06	-5.851	-5.907	-0.057	(0)	
FeOH+	2.564e-07	2.240e-07	-6.591	-6.650	-0.059	(0)	
Fe(OH)2	2.529e-11	2.529e-11	-10.597	-10.597	0.000	(0)	
Fe(OH)3-	3.088e-12	2.698e-12	-11.510	-11.569	-0.059	(0)	
Fe(3)	1.434e-04						
Fe(OH)2+	1.319e-04	1.155e-04	-3.880	-3.937	-0.058	(0)	
Fe(OH)3	9.615e-06	9.615e-06	-5.017	-5.017	0.000	(0)	
Fe(OH)4-	1.845e-06	1.615e-06	-5.734	-5.792	-0.058	(0)	
FeOH+2	7.230e-10	4.211e-10	-9.141	-9.376	-0.235	(0)	

FeSO4+ 6.046e-14 5.281e-14 -13.219 -13.277 -0.059 (0)
 Fe+3 1.145e-14 3.287e-15 -13.941 -14.483 -0.542 (0)
 Fe(SO4)2- 3.048e-15 2.579e-15 -14.516 -14.589 -0.073 (0)
 FeCl+2 2.128e-16 1.240e-16 -15.672 -15.907 -0.235 (0)
 Fe2(OH)2+4 1.262e-16 8.710e-18 -15.899 -17.060 -1.161 (0)
 FeCl2+ 1.590e-18 1.389e-18 -17.799 -17.857 -0.059 (0)
 Fe3(OH)4+5 8.447e-19 1.295e-20 -18.073 -19.888 -1.814 (0)
 FeNO3+2 1.391e-19 7.131e-20 -18.857 -19.147 -0.290 (0)
 FeHSeO3+2 1.218e-20 6.240e-21 -19.915 -20.205 -0.290 (0)
 FeCl3 2.457e-22 2.457e-22 -21.610 -21.610 0.000 (0)
 H(0) 1.141e-19
 H2 5.706e-20 5.734e-20 -19.244 -19.242 0.002 (0)
 K 1.034e-04
 K+ 1.020e-04 8.881e-05 -3.991 -4.052 -0.060 (0)
 KSO4- 1.412e-06 1.236e-06 -5.850 -5.908 -0.058 (0)
 Mg 1.882e-03
 Mg+2 1.537e-03 8.826e-04 -2.813 -3.054 -0.241 (0)
 MgSO4 3.077e-04 3.077e-04 -3.512 -3.512 0.000 (0)
 MgHCO3+ 3.425e-05 2.976e-05 -4.465 -4.526 -0.061 (0)
 MgCO3 2.991e-06 2.991e-06 -5.524 -5.524 0.000 (0)
 MgOH+ 5.341e-08 4.701e-08 -7.272 -7.328 -0.055 (0)
 MgUO2(CO3)3-2 5.518e-12 3.168e-12 -11.258 -11.499 -0.241 (0)
 Mn(2) 1.345e-05
 Mn+2 1.114e-05 5.709e-06 -4.953 -5.243 -0.290 (0)
 MnSO4 1.861e-06 1.861e-06 -5.730 -5.730 0.000 (0)
 MnHCO3+ 4.296e-07 3.753e-07 -6.367 -6.426 -0.059 (0)
 MnCl+ 1.456e-08 1.272e-08 -7.837 -7.896 -0.059 (0)
 MnOH+ 2.634e-09 2.301e-09 -8.579 -8.638 -0.059 (0)
 MnCl2 3.179e-11 3.179e-11 -10.498 -10.498 0.000 (0)
 MnNO3+ 1.324e-11 1.120e-11 -10.878 -10.951 -0.073 (0)
 MnCl3- 1.774e-14 1.550e-14 -13.751 -13.810 -0.059 (0)
 MnSe 2.529e-16 2.529e-16 -15.597 -15.597 0.000 (0)
 Mn(NO3)2 3.571e-17 3.571e-17 -16.447 -16.447 0.000 (0)
 Mn(OH)3- 5.306e-18 4.636e-18 -17.275 -17.334 -0.059 (0)
 Mn(OH)4-2 9.610e-24 5.597e-24 -23.017 -23.252 -0.235 (0)
 MnSeO4 1.557e-26 1.557e-26 -25.808 -25.808 0.000 (0)
 Mn(3) 5.482e-31
 Mn+3 5.482e-31 1.573e-31 -30.261 -30.803 -0.542 (0)
 Mn(6) 0.000e+00
 MnO4-2 0.000e+00 0.000e+00 -65.553 -65.788 -0.235 (0)
 Mn(7) 0.000e+00
 MnO4- 0.000e+00 0.000e+00 -75.331 -75.395 -0.064 (0)
 Mo 2.859e-07
 MoO4-2 2.858e-07 1.641e-07 -6.544 -6.785 -0.241 (0)
 HMoO4- 7.670e-11 6.490e-11 -10.115 -10.188 -0.073 (0)
 H2MoO4 2.570e-14 2.570e-14 -13.590 -13.590 0.000 (0)
 Mo7O24-6 0.000e+00 0.000e+00 -50.950 -53.562 -2.613 (0)
 HMo7O24-5 0.000e+00 0.000e+00 -52.997 -54.811 -1.814 (0)
 H2Mo7O24-4 0.000e+00 0.000e+00 -56.458 -57.619 -1.161 (0)
 H3Mo7O24-3 0.000e+00 0.000e+00 -61.277 -61.930 -0.653 (0)
 N(-3) 2.008e-05
 NH4+ 1.949e-05 1.678e-05 -4.710 -4.775 -0.065 (0)
 NH4SO4- 4.306e-07 3.762e-07 -6.366 -6.425 -0.059 (0)
 NH3 1.616e-07 1.616e-07 -6.791 -6.791 0.000 (0)
 CaNH3+2 1.280e-09 6.559e-10 -8.893 -9.183 -0.290 (0)
 Ca(NH3)2+2 1.811e-16 9.284e-17 -15.742 -16.032 -0.290 (0)
 N(5) 1.429e-06
 NO3- 1.422e-06 1.238e-06 -5.847 -5.907 -0.060 (0)
 CaNO3+ 7.358e-09 6.225e-09 -8.133 -8.206 -0.073 (0)
 MnNO3+ 1.324e-11 1.120e-11 -10.878 -10.951 -0.073 (0)
 Mn(NO3)2 3.571e-17 3.571e-17 -16.447 -16.447 0.000 (0)
 FeNO3+2 1.391e-19 7.131e-20 -18.857 -19.147 -0.290 (0)
 UO2NO3+ 1.028e-23 8.701e-24 -22.988 -23.060 -0.073 (0)
 Na 4.271e-03
 Na+ 4.216e-03 3.670e-03 -2.375 -2.435 -0.060 (0)
 NaSO4- 4.638e-05 4.060e-05 -4.334 -4.391 -0.058 (0)

NaHCO3	8.897e-06	8.897e-06	-5.051	-5.051	0.000	(0)
NaCO3-	5.194e-07	4.547e-07	-6.285	-6.342	-0.058	(0)
O(0)	1.251e-05					
O2	6.256e-06	6.287e-06	-5.204	-5.202	0.002	(0)
S(6)	4.647e-03					
SO4-2	3.643e-03	2.092e-03	-2.439	-2.679	-0.241	(0)
CaSO4	6.306e-04	6.306e-04	-3.200	-3.200	0.000	(0)
MgSO4	3.077e-04	3.077e-04	-3.512	-3.512	0.000	(0)
NaSO4-	4.638e-05	4.060e-05	-4.334	-4.391	-0.058	(0)
FeSO4	1.595e-05	1.595e-05	-4.797	-4.797	0.000	(0)
MnSO4	1.861e-06	1.861e-06	-5.730	-5.730	0.000	(0)
KSO4-	1.412e-06	1.236e-06	-5.850	-5.908	-0.058	(0)
NH4SO4-	4.306e-07	3.762e-07	-6.366	-6.425	-0.059	(0)
HSO4-	4.524e-09	3.942e-09	-8.345	-8.404	-0.060	(0)
FeSO4+	6.046e-14	5.281e-14	-13.219	-13.277	-0.059	(0)
Fe(SO4)2-	3.048e-15	2.579e-15	-14.516	-14.589	-0.073	(0)
UO2SO4	6.866e-18	6.866e-18	-17.163	-17.163	0.000	(0)
UO2(SO4)2-2	2.812e-19	1.441e-19	-18.551	-18.841	-0.290	(0)
U(SO4)2	1.891e-34	1.891e-34	-33.723	-33.723	0.000	(0)
USO4+2	3.244e-35	1.663e-35	-34.489	-34.779	-0.290	(0)
Se(-2)	3.423e-13					
HSe-	3.419e-13	2.893e-13	-12.466	-12.539	-0.073	(0)
MnSe	2.529e-16	2.529e-16	-15.597	-15.597	0.000	(0)
H2Se	5.750e-17	5.750e-17	-16.240	-16.240	0.000	(0)
Se-2	1.011e-20	5.183e-21	-19.995	-20.285	-0.290	(0)
Se(4)	1.521e-09					
HSeO3-	1.240e-09	1.049e-09	-8.906	-8.979	-0.073	(0)
SeO3-2	2.807e-10	1.438e-10	-9.552	-9.842	-0.290	(0)
H2SeO3	1.097e-14	1.097e-14	-13.960	-13.960	0.000	(0)
FeHSeO3+2	1.218e-20	6.240e-21	-19.915	-20.205	-0.290	(0)
Se(6)	2.184e-23					
SeO4-2	2.183e-23	1.253e-23	-22.661	-22.902	-0.241	(0)
MnSeO4	1.557e-26	1.557e-26	-25.808	-25.808	0.000	(0)
HSeO4-	1.410e-29	1.193e-29	-28.851	-28.923	-0.073	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-47.962	-48.615	-0.653	(0)
U(4)	2.487e-15					
U(OH)5-	2.484e-15	2.102e-15	-14.605	-14.677	-0.073	(0)
U(OH)4	2.833e-18	2.833e-18	-17.548	-17.548	0.000	(0)
U(OH)3+	3.769e-22	3.189e-22	-21.424	-21.496	-0.073	(0)
U(OH)2+2	1.058e-26	5.423e-27	-25.975	-26.266	-0.290	(0)
UOH+3	4.615e-32	1.026e-32	-31.336	-31.989	-0.653	(0)
U(SO4)2	1.891e-34	1.891e-34	-33.723	-33.723	0.000	(0)
USO4+2	3.244e-35	1.663e-35	-34.489	-34.779	-0.290	(0)
U+4	3.267e-38	2.254e-39	-37.486	-38.647	-1.161	(0)
UCl+3	1.218e-39	2.707e-40	-38.914	-39.567	-0.653	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-129.611	-135.489	-5.878	(0)
U(5)	8.247e-16					
UO2+	8.247e-16	6.978e-16	-15.084	-15.156	-0.073	(0)
U(6)	5.047e-09					
Ca2UO2(CO3)3	3.672e-09	3.689e-09	-8.435	-8.433	0.002	(0)
CaUO2(CO3)3-2	1.324e-09	7.604e-10	-8.878	-9.119	-0.241	(0)
UO2(CO3)3-4	3.627e-11	2.503e-12	-10.440	-11.602	-1.161	(0)
UO2(CO3)2-2	8.530e-12	4.372e-12	-11.069	-11.359	-0.290	(0)
MgUO2(CO3)3-2	5.518e-12	3.168e-12	-11.258	-11.499	-0.241	(0)
UO2(OH)2	1.954e-13	1.963e-13	-12.709	-12.707	0.002	(0)
UO2CO3	5.378e-14	5.378e-14	-13.269	-13.269	0.000	(0)
UO2(OH)3-	1.037e-14	9.029e-15	-13.984	-14.044	-0.060	(0)
UO2OH+	7.916e-17	6.698e-17	-16.101	-16.174	-0.073	(0)
UO2SO4	6.866e-18	6.866e-18	-17.163	-17.163	0.000	(0)
UO2+2	5.115e-18	2.937e-18	-17.291	-17.532	-0.241	(0)
(UO2)2CO3(OH)3-	3.952e-19	3.440e-19	-18.403	-18.463	-0.060	(0)
UO2(SO4)2-2	2.812e-19	1.441e-19	-18.551	-18.841	-0.290	(0)
UO2(OH)4-2	9.102e-21	5.226e-21	-20.041	-20.282	-0.241	(0)
UO2Cl+	7.816e-21	6.613e-21	-20.107	-20.180	-0.073	(0)
UO2NO3+	1.028e-23	8.701e-24	-22.988	-23.060	-0.073	(0)

UO2Cl2 6.859e-25 6.892e-25 -24.164 -24.162 0.002 (0)
 (UO2)2(OH)2+2 3.284e-26 1.683e-26 -25.484 -25.774 -0.290 (0)
 (UO2)3(CO3)6-6 1.575e-28 1.068e-30 -27.803 -29.971 -2.169 (0)
 (UO2)2OH+3 2.191e-30 6.287e-31 -29.659 -30.202 -0.542 (0)
 (UO2)3(OH)7- 2.524e-31 2.197e-31 -30.598 -30.658 -0.060 (0)
 (UO2)3(OH)5+ 1.069e-31 9.046e-32 -30.971 -31.044 -0.073 (0)
 (UO2)3(OH)4+2 9.886e-35 5.676e-35 -34.005 -34.246 -0.241 (0)
 (UO2)4(OH)7+ 9.331e-40 8.123e-40 -39.030 -39.090 -0.060 (0)

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

Phase	SI**	log IAP	log K(287 K, 1 atm)
(NH4)2SeO4	-32.90	-32.45	0.45 (NH4)2SeO4
Anhydrite	-1.20	-5.51	-4.31 CaSO4
Aragonite	0.08	-8.14	-8.22 CaCO3
Artinite	-6.67	3.72	10.39 MgCO3:Mg(OH)2:3H2O
Birnessite	-18.11	-0.02	18.09 MnO2
Bixbyite	-16.36	-16.19	0.18 Mn2O3
Brucite	-5.51	12.09	17.59 Mg(OH)2
Calcite	0.28	-8.14	-8.43 CaCO3
CaMoO4	-1.68	-9.62	-7.94 CaMoO4
CaSeO3:2H2O	-7.19	-4.24	2.94 CaSeO3:2H2O
CaSeO4:2H2O	-22.77	-25.74	-2.97 CaSeO4:2H2O
CH4(g)	-42.27	-85.01	-42.74 CH4
CO2(g)	-2.28	-20.45	-18.17 CO2
Dolomite(disordered)	-0.28	-16.51	-16.23 CaMg(CO3)2
Dolomite(ordered)	0.32	-16.51	-16.83 CaMg(CO3)2
Epsomite	-3.53	-5.73	-2.20 MgSO4:7H2O
Fe(OH)2	-2.88	10.68	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	8.17	5.13	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-1.65	-0.10	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-12.57	-33.19	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-34.86	-37.00	-2.14 Fe2(SO4)3
Fe3(OH)8	6.92	27.14	20.22 Fe3(OH)8
FeMoO4	-1.22	-11.24	-10.02 FeMoO4
Ferrihydrite	4.55	8.23	3.67 Fe(OH)3
Ferroselite	5.51	-13.39	-18.91 FeSe2
FeSe	1.59	-9.42	-11.01 FeSe
Goethite	7.34	8.23	0.89 FeOOH
Gummite	-10.60	-2.39	8.21 UO3
Gypsum	-0.90	-5.51	-4.62 CaSO4:2H2O
H-Jarosite	-0.38	-10.96	-10.58 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-8.73	-21.92	-13.20 H2MoO4
H2Se(g)	-15.25	-20.11	-4.86 H2Se
Halite	-6.77	-5.19	1.58 NaCl
Hausmannite	-17.97	45.83	63.80 Mn3O4
Hematite	17.02	16.45	-0.57 Fe2O3
Huntite	-3.98	-33.24	-29.26 CaMg3(CO3)4
Hydromagnesite	-14.05	-21.38	-7.33 Mg5(CO3)4(OH)2:4H2O
K-Jarosite	6.50	-7.44	-13.94 KFe3(SO4)2(OH)6
K2MoO4	-18.17	-14.89	3.28 K2MoO4
K2SeO4	-30.28	-31.01	-0.73 K2SeO4
Lepidocrocite	6.86	8.23	1.37 FeOOH
Lime	-21.67	12.31	33.98 CaO
Maghemite	10.07	16.45	6.39 Fe2O3
Magnesianoferrite	9.84	28.54	18.70 Fe2MgO4
Magnesite	-0.77	-8.37	-7.59 MgCO3
Magnetite	22.36	27.14	4.78 Fe3O4
Manganite	-7.37	17.97	25.34 MnOOH
Melanterite	-4.79	-7.14	-2.34 FeSO4:7H2O
Mg(OH)2(active)	-6.71	12.09	18.79 Mg(OH)2
MgMoO4	-7.99	-9.84	-1.85 MgMoO4
MgSeO3:6H2O	-7.49	-4.46	3.02 MgSeO3:6H2O
MgSeO4:6H2O	-24.76	-25.96	-1.20 MgSeO4:6H2O
Mirabilite	-5.91	-7.55	-1.64 Na2SO4:10H2O

Mn2(SO4)3 -65.01 -69.64 -4.63 Mn2(SO4)3
MnCl2:4H2O -13.53 -10.75 2.79 MnCl2:4H2O
MnSe -14.36 -10.21 4.15 MnSe
MnSeO3 -7.78 -6.65 1.13 MnSeO3
MnSeO3:2H2O -7.58 -6.65 0.93 MnSeO3:2H2O
MnSeO4:5H2O -26.10 -28.15 -2.05 MnSeO4:5H2O
MnSO4 -10.93 -7.92 3.01 MnSO4
MoO3 -13.92 -21.92 -8.00 MoO3
Na-Jarosite 4.38 -5.82 -10.20 NaFe3(SO4)2(OH)6
Na2Mo2O7 -16.61 -33.58 -16.97 Na2Mo2O7
Na2MoO4 -13.21 -11.66 1.56 Na2MoO4
Na2MoO4:2H2O -12.88 -11.66 1.22 Na2MoO4:2H2O
Na2SeO3:5H2O -16.58 -6.28 10.30 Na2SeO3:5H2O
Na2SeO4 -29.05 -27.77 1.28 Na2SeO4
Natron -8.44 -10.18 -1.74 Na2CO3:10H2O
Nesquehonite -3.86 -8.37 -4.51 MgCO3:3H2O
Nsutite -17.53 -0.02 17.50 MnO2
O2(g) -54.57 32.28 86.85 O2
Periclase -10.49 12.09 22.58 MgO
Portlandite -11.35 12.31 23.65 Ca(OH)2
Pyrochroite -5.94 9.90 15.83 Mn(OH)2
Pyrolusite -17.13 26.04 43.17 MnO2
Rhodochrosite 0.01 -10.55 -10.57 MnCO3
Rutherfordine -8.36 -22.84 -14.48 UO2CO3
Schoepite -8.71 -2.39 6.32 UO2(OH)2:H2O
Semetal(am) 3.21 -3.97 -7.18 Se
Semetal(hex) 3.84 -3.97 -7.81 Se
SeO2 -16.66 -16.55 0.12 SeO2
SeO3 -60.05 -38.04 22.01 SeO3
Siderite 0.37 -9.77 -10.13 FeCO3
Thenardite -7.93 -7.55 0.38 Na2SO4
Thermonatrite -10.89 -10.18 0.71 Na2CO3:H2O
U3O8 -17.10 7.18 24.28 U3O8
U4O9 -17.12 -17.33 -0.21 U4O9
UO2(am) -10.02 -8.37 1.66 UO2
UO2(NO3)2 -42.04 -29.35 12.70 UO2(NO3)2
UO2(NO3)2:2H2O -34.37 -29.35 5.02 UO2(NO3)2:2H2O
UO2(NO3)2:3H2O -32.80 -29.35 3.45 UO2(NO3)2:3H2O
UO2(NO3)2:6H2O -31.26 -29.35 1.91 UO2(NO3)2:6H2O
UO2(OH)2(beta) -8.38 -2.39 5.99 UO2(OH)2
UO2SeO4:4H2O -38.18 -40.43 -2.25 UO2SeO4:4H2O
UO3 -10.63 -2.39 8.23 UO3
Uraninite -4.21 -8.37 -4.16 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 14. SAG1-2

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

Elements	Molality	Moles
Alkalinity	4.581e-03	4.581e-03
Ca	3.772e-03	3.772e-03
Cl	2.440e-03	2.440e-03
Fe(2)	1.703e-05	1.703e-05
Fe(3)	1.076e-06	1.076e-06
K	1.232e-04	1.232e-04
Mg	2.043e-03	2.043e-03
Mn	7.654e-05	7.654e-05
Mo	2.024e-07	2.024e-07
N(-3)	5.618e-05	5.618e-05
N(5)	1.429e-06	1.429e-06
Na	5.313e-03	5.313e-03
O(0)	1.189e-05	1.189e-05

S(6) 4.940e-03 4.940e-03
 Se 1.268e-09 1.268e-09
 U 2.784e-08 2.784e-08

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

pH = 7.760
 pe = 2.100
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.321e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 4.713e-03
 Total CO2 (mol/kg) = 4.713e-03
 Temperature (°C) = 13.90
 Electrical balance (eq) = 4.081e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.39
 Iterations = 12 (244 overall)
 Total H = 1.110187e+02
 Total O = 5.554075e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	1.4830	0.0845
N(-3)/N(5)	5.6503	0.3218
O(-2)/O(0)	13.2478	0.7545

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	2.817e-07	2.425e-07	-6.550	-6.615	-0.065	(0)	
H+	2.008e-08	1.738e-08	-7.697	-7.760	-0.063	0.00	
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.03	
C(4)	4.713e-03						
HCO3-	4.353e-03	3.790e-03	-2.361	-2.421	-0.060	(0)	
H2CO3	1.709e-04	1.709e-04	-3.767	-3.767	0.000	(0)	
CaHCO3+	9.743e-05	8.510e-05	-4.011	-4.070	-0.059	(0)	
MgHCO3+	3.944e-05	3.407e-05	-4.404	-4.468	-0.064	(0)	
CaCO3	1.656e-05	1.656e-05	-4.781	-4.781	0.000	(0)	
CO3-2	1.451e-05	8.142e-06	-4.838	-5.089	-0.251	(0)	
NaHCO3	1.198e-05	1.198e-05	-4.922	-4.922	0.000	(0)	
MgCO3	5.251e-06	5.251e-06	-5.280	-5.280	0.000	(0)	
MnHCO3+	2.568e-06	2.231e-06	-5.590	-5.651	-0.061	(0)	
NaCO3-	1.085e-06	9.446e-07	-5.965	-6.025	-0.060	(0)	
FeHCO3+	2.920e-07	2.550e-07	-6.535	-6.593	-0.059	(0)	
Ca2UO2(CO3)3	2.078e-08	2.089e-08	-7.682	-7.680	0.002	(0)	
CaUO2(CO3)3-2	6.824e-09	3.830e-09	-8.166	-8.417	-0.251	(0)	
UO2(CO3)3-4	1.898e-10	1.141e-11	-9.722	-10.943	-1.221	(0)	
MgUO2(CO3)3-2	2.679e-11	1.504e-11	-10.572	-10.823	-0.251	(0)	
UO2(CO3)2-2	2.358e-11	1.167e-11	-10.628	-10.933	-0.305	(0)	
UO2CO3	8.665e-14	8.665e-14	-13.062	-13.062	0.000	(0)	
(UO2)2CO3(OH)3-	2.324e-18	2.011e-18	-17.634	-17.696	-0.063	(0)	
(UO2)3(CO3)6-6	3.913e-27	2.159e-29	-26.407	-28.666	-2.258	(0)	
Ca	3.772e-03						
Ca+2	2.936e-03	1.647e-03	-2.532	-2.783	-0.251	(0)	
CaSO4	7.222e-04	7.222e-04	-3.141	-3.141	0.000	(0)	
CaHCO3+	9.743e-05	8.510e-05	-4.011	-4.070	-0.059	(0)	
CaCO3	1.656e-05	1.656e-05	-4.781	-4.781	0.000	(0)	
Ca2UO2(CO3)3	2.078e-08	2.089e-08	-7.682	-7.680	0.002	(0)	
CaNO3+	8.309e-09	6.970e-09	-8.080	-8.157	-0.076	(0)	
CaOH+	8.018e-09	7.003e-09	-8.096	-8.155	-0.059	(0)	
CaUO2(CO3)3-2	6.824e-09	3.830e-09	-8.166	-8.417	-0.251	(0)	
CaNH3+2	6.379e-09	3.159e-09	-8.195	-8.501	-0.305	(0)	

Ca(NH3)2+2 3.868e-15 1.915e-15 -14.413 -14.718 -0.305 (0)
 Cl 2.440e-03
 Cl- 2.440e-03 2.112e-03 -2.613 -2.675 -0.063 (0)
 MnCl+ 9.610e-08 8.349e-08 -7.017 -7.078 -0.061 (0)
 MnCl2 2.490e-10 2.490e-10 -9.604 -9.604 0.000 (0)
 MnCl3- 1.667e-13 1.448e-13 -12.778 -12.839 -0.061 (0)
 FeCl+2 7.617e-19 4.339e-19 -18.118 -18.363 -0.244 (0)
 UO2Cl+ 9.050e-21 7.592e-21 -20.043 -20.120 -0.076 (0)
 FeCl2+ 6.744e-21 5.859e-21 -20.171 -20.232 -0.061 (0)
 FeCl3 1.237e-24 1.237e-24 -23.908 -23.908 0.000 (0)
 UO2Cl2 9.456e-25 9.507e-25 -24.024 -24.022 0.002 (0)
 UCl+3 0.000e+00 0.000e+00 -42.747 -43.433 -0.687 (0)
 Fe(2) 1.703e-05
 Fe+2 1.355e-05 6.712e-06 -4.868 -5.173 -0.305 (0)
 FeSO4 3.109e-06 3.109e-06 -5.507 -5.507 0.000 (0)
 FeHCO3+ 2.920e-07 2.550e-07 -6.535 -6.593 -0.059 (0)
 FeOH+ 7.459e-08 6.480e-08 -7.127 -7.188 -0.061 (0)
 Fe(OH)2 1.102e-11 1.102e-11 -10.958 -10.958 0.000 (0)
 Fe(OH)3- 2.089e-12 1.815e-12 -11.680 -11.741 -0.061 (0)
 Fe(3) 1.076e-06
 Fe(OH)2+ 9.428e-07 8.209e-07 -6.026 -6.086 -0.060 (0)
 Fe(OH)3 1.011e-07 1.011e-07 -6.995 -6.995 0.000 (0)
 Fe(OH)4- 3.163e-08 2.754e-08 -7.500 -7.560 -0.060 (0)
 FeOH+2 3.331e-12 1.898e-12 -11.477 -11.722 -0.244 (0)
 FeSO4+ 1.821e-16 1.582e-16 -15.740 -15.801 -0.061 (0)
 Fe+3 3.574e-17 9.741e-18 -16.447 -17.011 -0.565 (0)
 Fe(SO4)2- 9.437e-18 7.916e-18 -17.025 -17.101 -0.076 (0)
 FeCl+2 7.617e-19 4.339e-19 -18.118 -18.363 -0.244 (0)
 FeCl2+ 6.744e-21 5.859e-21 -20.171 -20.232 -0.061 (0)
 Fe2(OH)2+4 2.975e-21 1.789e-22 -20.527 -21.747 -1.221 (0)
 FeNO3+2 4.309e-22 2.134e-22 -21.366 -21.671 -0.305 (0)
 FeHSeO3+2 2.755e-23 1.364e-23 -22.560 -22.865 -0.305 (0)
 FeCl3 1.237e-24 1.237e-24 -23.908 -23.908 0.000 (0)
 Fe3(OH)4+5 1.524e-25 1.885e-27 -24.817 -26.725 -1.908 (0)
 H(0) 3.010e-23
 H2 1.505e-23 1.513e-23 -22.822 -22.820 0.002 (0)
 K 1.232e-04
 K+ 1.214e-04 1.051e-04 -3.916 -3.978 -0.063 (0)
 KSO4- 1.714e-06 1.492e-06 -5.766 -5.826 -0.060 (0)
 Mg 2.043e-03
 Mg+2 1.666e-03 9.349e-04 -2.778 -3.029 -0.251 (0)
 MgSO4 3.322e-04 3.322e-04 -3.479 -3.479 0.000 (0)
 MgHCO3+ 3.944e-05 3.407e-05 -4.404 -4.468 -0.064 (0)
 MgCO3 5.251e-06 5.251e-06 -5.280 -5.280 0.000 (0)
 MgOH+ 8.548e-08 7.485e-08 -7.068 -7.126 -0.058 (0)
 MgUO2(CO3)3-2 2.679e-11 1.504e-11 -10.572 -10.823 -0.251 (0)
 Mn(2) 7.654e-05
 Mn+2 6.342e-05 3.141e-05 -4.198 -4.503 -0.305 (0)
 MnSO4 1.042e-05 1.042e-05 -4.982 -4.982 0.000 (0)
 MnHCO3+ 2.568e-06 2.231e-06 -5.590 -5.651 -0.061 (0)
 MnCl+ 9.610e-08 8.349e-08 -7.017 -7.078 -0.061 (0)
 MnOH+ 2.202e-08 1.913e-08 -7.657 -7.718 -0.061 (0)
 MnCl2 2.490e-10 2.490e-10 -9.604 -9.604 0.000 (0)
 MnNO3+ 7.298e-11 6.122e-11 -10.137 -10.213 -0.076 (0)
 MnCl3- 1.667e-13 1.448e-13 -12.778 -12.839 -0.061 (0)
 Mn(NO3)2 1.941e-16 1.941e-16 -15.712 -15.712 0.000 (0)
 Mn(OH)3- 1.091e-16 9.474e-17 -15.962 -16.023 -0.061 (0)
 MnSeO4 3.425e-22 3.425e-22 -21.465 -21.465 0.000 (0)
 Mn(OH)4-2 3.110e-22 1.772e-22 -21.507 -21.752 -0.244 (0)
 MnSe 2.925e-26 2.925e-26 -25.534 -25.534 0.000 (0)
 Mn(3) 1.206e-28
 Mn+3 1.206e-28 3.287e-29 -27.919 -28.483 -0.565 (0)
 Mn(6) 0.000e+00
 MnO4-2 0.000e+00 0.000e+00 -57.018 -57.263 -0.244 (0)
 Mn(7) 0.000e+00
 MnO4- 0.000e+00 0.000e+00 -65.224 -65.291 -0.066 (0)

Mo 2.024e-07
 MoO4-2 2.024e-07 1.136e-07 -6.694 -6.945 -0.251 (0)
 HMoO4- 3.427e-11 2.875e-11 -10.465 -10.541 -0.076 (0)
 H2MoO4 7.499e-15 7.499e-15 -14.125 -14.125 0.000 (0)
 Mo7O24-6 0.000e+00 0.000e+00 -53.411 -56.158 -2.747 (0)
 HMo7O24-5 0.000e+00 0.000e+00 -55.691 -57.599 -1.908 (0)
 H2Mo7O24-4 0.000e+00 0.000e+00 -59.376 -60.597 -1.221 (0)
 H3Mo7O24-3 0.000e+00 0.000e+00 -64.410 -65.097 -0.687 (0)
 N(-3) 5.618e-05
 NH4+ 5.427e-05 4.642e-05 -4.265 -4.333 -0.068 (0)
 NH4SO4- 1.224e-06 1.063e-06 -5.912 -5.973 -0.061 (0)
 NH3 6.768e-07 6.768e-07 -6.170 -6.170 0.000 (0)
 CaNH3+2 6.379e-09 3.159e-09 -8.195 -8.501 -0.305 (0)
 Ca(NH3)2+2 3.868e-15 1.915e-15 -14.413 -14.718 -0.305 (0)
 N(5) 1.429e-06
 NO3- 1.421e-06 1.230e-06 -5.847 -5.910 -0.063 (0)
 CaNO3+ 8.309e-09 6.970e-09 -8.080 -8.157 -0.076 (0)
 MnNO3+ 7.298e-11 6.122e-11 -10.137 -10.213 -0.076 (0)
 Mn(NO3)2 1.941e-16 1.941e-16 -15.712 -15.712 0.000 (0)
 FeNO3+2 4.309e-22 2.134e-22 -21.366 -21.671 -0.305 (0)
 UO2NO3+ 1.004e-23 8.420e-24 -22.998 -23.075 -0.076 (0)
 Na 5.313e-03
 Na+ 5.241e-03 4.536e-03 -2.281 -2.343 -0.063 (0)
 NaSO4- 5.889e-05 5.127e-05 -4.230 -4.290 -0.060 (0)
 NaHCO3 1.198e-05 1.198e-05 -4.922 -4.922 0.000 (0)
 NaCO3- 1.085e-06 9.446e-07 -5.965 -6.025 -0.060 (0)
 O(0) 1.189e-05
 O2 5.944e-06 5.976e-06 -5.226 -5.224 0.002 (0)
 S(6) 4.940e-03
 SO4-2 3.810e-03 2.138e-03 -2.419 -2.670 -0.251 (0)
 CaSO4 7.222e-04 7.222e-04 -3.141 -3.141 0.000 (0)
 MgSO4 3.322e-04 3.322e-04 -3.479 -3.479 0.000 (0)
 NaSO4- 5.889e-05 5.127e-05 -4.230 -4.290 -0.060 (0)
 MnSO4 1.042e-05 1.042e-05 -4.982 -4.982 0.000 (0)
 FeSO4 3.109e-06 3.109e-06 -5.507 -5.507 0.000 (0)
 KSO4- 1.714e-06 1.492e-06 -5.766 -5.826 -0.060 (0)
 NH4SO4- 1.224e-06 1.063e-06 -5.912 -5.973 -0.061 (0)
 HSO4- 2.974e-09 2.576e-09 -8.527 -8.589 -0.062 (0)
 FeSO4+ 1.821e-16 1.582e-16 -15.740 -15.801 -0.061 (0)
 Fe(SO4)2- 9.437e-18 7.916e-18 -17.025 -17.101 -0.076 (0)
 UO2SO4 6.739e-18 6.739e-18 -17.171 -17.171 0.000 (0)
 UO2(SO4)2-2 2.897e-19 1.434e-19 -18.538 -18.843 -0.305 (0)
 U(SO4)2 2.203e-38 2.203e-38 -37.657 -37.657 0.000 (0)
 USO4+2 3.870e-39 1.916e-39 -38.412 -38.718 -0.305 (0)
 Se(-2) 4.711e-24
 HSe- 4.682e-24 3.927e-24 -23.330 -23.406 -0.076 (0)
 MnSe 2.925e-26 2.925e-26 -25.534 -25.534 0.000 (0)
 H2Se 5.032e-28 5.032e-28 -27.298 -27.298 0.000 (0)
 Se-2 2.155e-31 1.067e-31 -30.667 -30.972 -0.305 (0)
 Se(4) 1.268e-09
 HSeO3- 9.331e-10 7.827e-10 -9.030 -9.106 -0.076 (0)
 SeO3-2 3.348e-10 1.658e-10 -9.475 -9.780 -0.305 (0)
 H2SeO3 5.267e-15 5.267e-15 -14.278 -14.278 0.000 (0)
 FeHSeO3+2 2.755e-23 1.364e-23 -22.560 -22.865 -0.305 (0)
 Se(6) 9.016e-20
 SeO4-2 8.982e-20 5.040e-20 -19.047 -19.298 -0.251 (0)
 MnSeO4 3.425e-22 3.425e-22 -21.465 -21.465 0.000 (0)
 HSeO4- 3.655e-26 3.066e-26 -25.437 -25.513 -0.076 (0)
 U(3) 0.000e+00
 U+3 0.000e+00 0.000e+00 -53.494 -54.181 -0.687 (0)
 U(4) 2.404e-18
 U(OH)5- 2.402e-18 2.015e-18 -17.619 -17.696 -0.076 (0)
 U(OH)4 1.763e-21 1.763e-21 -20.754 -20.754 0.000 (0)
 U(OH)3+ 1.533e-25 1.286e-25 -24.814 -24.891 -0.076 (0)
 U(OH)2+2 2.877e-30 1.425e-30 -29.541 -29.846 -0.305 (0)
 UOH+3 8.558e-36 1.760e-36 -35.068 -35.754 -0.687 (0)

U(SO4)2 2.203e-38 2.203e-38 -37.657 -37.657 0.000 (0)
 USO4+2 3.870e-39 1.916e-39 -38.412 -38.718 -0.305 (0)
 U+4 0.000e+00 0.000e+00 -41.372 -42.593 -1.221 (0)
 UCl+3 0.000e+00 0.000e+00 -42.747 -43.433 -0.687 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -150.137 -156.318 -6.181 (0)
 U(5) 2.037e-17
 UO2+ 2.037e-17 1.708e-17 -16.691 -16.767 -0.076 (0)
 U(6) 2.784e-08
 Ca2UO2(CO3)3 2.078e-08 2.089e-08 -7.682 -7.680 0.002 (0)
 CaUO2(CO3)3-2 6.824e-09 3.830e-09 -8.166 -8.417 -0.251 (0)
 UO2(CO3)3-4 1.898e-10 1.141e-11 -9.722 -10.943 -1.221 (0)
 MgUO2(CO3)3-2 2.679e-11 1.504e-11 -10.572 -10.823 -0.251 (0)
 UO2(CO3)2-2 2.358e-11 1.167e-11 -10.628 -10.933 -0.305 (0)
 UO2(OH)2 4.538e-13 4.562e-13 -12.343 -12.341 0.002 (0)
 UO2CO3 8.665e-14 8.665e-14 -13.062 -13.062 0.000 (0)
 UO2(OH)3- 3.755e-14 3.250e-14 -13.425 -13.488 -0.063 (0)
 UO2OH+ 1.173e-16 9.842e-17 -15.931 -16.007 -0.076 (0)
 UO2SO4 6.739e-18 6.739e-18 -17.171 -17.171 0.000 (0)
 UO2+2 5.070e-18 2.845e-18 -17.295 -17.546 -0.251 (0)
 (UO2)2CO3(OH)3- 2.324e-18 2.011e-18 -17.634 -17.696 -0.063 (0)
 UO2(SO4)2-2 2.897e-19 1.434e-19 -18.538 -18.843 -0.305 (0)
 UO2(OH)4-2 5.191e-20 2.913e-20 -19.285 -19.536 -0.251 (0)
 UO2Cl+ 9.050e-21 7.592e-21 -20.043 -20.120 -0.076 (0)
 UO2NO3+ 1.004e-23 8.420e-24 -22.998 -23.075 -0.076 (0)
 UO2Cl2 9.456e-25 9.507e-25 -24.024 -24.022 0.002 (0)
 (UO2)2(OH)2+2 7.513e-26 3.721e-26 -25.124 -25.429 -0.305 (0)
 (UO2)3(CO3)6-6 3.913e-27 2.159e-29 -26.407 -28.666 -2.258 (0)
 (UO2)3(OH)7- 4.933e-30 4.270e-30 -29.307 -29.370 -0.063 (0)
 (UO2)2OH+3 3.353e-30 9.139e-31 -29.475 -30.039 -0.565 (0)
 (UO2)3(OH)5+ 8.335e-31 6.992e-31 -30.079 -30.155 -0.076 (0)
 (UO2)3(OH)4+2 5.292e-34 2.970e-34 -33.276 -33.527 -0.251 (0)
 (UO2)4(OH)7+ 1.767e-38 1.529e-38 -37.753 -37.815 -0.063 (0)

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

Phase	SI**	log IAP	log K(287 K, 1 atm)
(NH4)2SeO4	-28.41	-27.96	0.45 (NH4)2SeO4
Anhydrite	-1.14	-5.45	-4.31 CaSO4
Aragonite	0.35	-7.87	-8.22 CaCO3
Artinite	-6.04	4.37	10.41 MgCO3:Mg(OH)2:3H2O
Birnessite	-13.43	4.66	18.09 MnO2
Bixbyite	-10.61	-10.41	0.20 Mn2O3
Brucite	-5.13	12.49	17.62 Mg(OH)2
Calcite	0.55	-7.87	-8.43 CaCO3
CaMoO4	-1.79	-9.73	-7.94 CaMoO4
CaSeO3:2H2O	-7.08	-4.13	2.95 CaSeO3:2H2O
CaSeO4:2H2O	-19.12	-22.08	-2.96 CaSeO4:2H2O
CH4(g)	-56.70	-99.49	-42.79 CH4
CO2(g)	-2.43	-20.61	-18.17 CO2
Dolomite(disordered)	0.23	-15.99	-16.23 CaMg(CO3)2
Dolomite(ordered)	0.83	-15.99	-16.82 CaMg(CO3)2
Epsomite	-3.50	-5.70	-2.20 MgSO4:7H2O
Fe(OH)2	-3.22	10.35	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	6.18	3.14	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-5.88	-4.33	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-17.44	-38.06	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-39.94	-42.03	-2.09 Fe2(SO4)3
Fe3(OH)8	2.66	22.88	20.22 Fe3(OH)8
FeMoO4	-2.10	-12.12	-10.02 FeMoO4
Ferrihydrite	2.58	6.27	3.69 Fe(OH)3
Ferroselite	-13.35	-32.26	-18.92 FeSe2
FeSe	-9.80	-20.82	-11.01 FeSe
Goethite	5.37	6.27	0.90 FeOOH
Gummitte	-10.25	-2.03	8.22 UO3
Gypsum	-0.84	-5.45	-4.62 CaSO4:2H2O

H-Jarosite -7.04 -17.58 -10.54 (H3O)Fe3(SO4)2(OH)6
H2MoO4 -9.26 -22.46 -13.21 H2MoO4
H2Se(g) -26.31 -31.17 -4.86 H2Se
Halite -6.60 -5.02 1.58 NaCl
Hausmannite -11.11 52.77 63.88 Mn3O4
Hematite 13.08 12.54 -0.54 Fe2O3
Huntite -2.99 -32.23 -29.24 CaMg3(CO3)4
Hydromagnesite -12.70 -19.98 -7.29 Mg5(CO3)4(OH)2·4H2O
K-Jarosite 0.12 -13.79 -13.91 KFe3(SO4)2(OH)6
K2MoO4 -18.19 -14.90 3.28 K2MoO4
K2SeO4 -26.52 -27.25 -0.73 K2SeO4
Lepidocrocite 4.90 6.27 1.37 FeOOH
Lime -21.28 12.74 34.01 CaO
Maghemite 6.15 12.54 6.39 Fe2O3
Magnesioferrite 6.28 25.03 18.75 Fe2MgO4
Magnesite -0.52 -8.12 -7.60 MgCO3
Magnetite 18.07 22.88 4.82 Fe3O4
Manganite -4.46 20.88 25.34 MnOOH
Melanterite -5.50 -7.84 -2.35 FeSO4·7H2O
Mg(OH)2(active) -6.30 12.49 18.79 Mg(OH)2
MgMoO4 -8.12 -9.97 -1.85 MgMoO4
MgSeO3·6H2O -7.40 -4.38 3.02 MgSeO3·6H2O
MgSeO4·6H2O -21.13 -22.33 -1.20 MgSeO4·6H2O
Mirabilite -5.71 -7.36 -1.65 Na2SO4·10H2O
Mn2(SO4)3 -60.37 -64.98 -4.60 Mn2(SO4)3
MnCl2·4H2O -12.64 -9.85 2.79 MnCl2·4H2O
MnSe -24.31 -20.15 4.16 MnSe
MnSeO3 -6.98 -5.85 1.13 MnSeO3
MnSeO3·2H2O -6.77 -5.85 0.92 MnSeO3·2H2O
MnSeO4·5H2O -21.75 -23.80 -2.05 MnSeO4·5H2O
MnSO4 -10.20 -7.17 3.02 MnSO4
MoO3 -14.46 -22.46 -8.00 MoO3
Na-Jarosite -1.98 -12.16 -10.17 NaFe3(SO4)2(OH)6
Na2Mo2O7 -17.12 -34.10 -16.98 Na2Mo2O7
Na2MoO4 -13.19 -11.63 1.56 Na2MoO4
Na2MoO4·2H2O -12.86 -11.63 1.22 Na2MoO4·2H2O
Na2SeO3·5H2O -16.33 -6.03 10.30 Na2SeO3·5H2O
Na2SeO4 -25.26 -23.98 1.28 Na2SeO4
Natron -8.02 -9.78 -1.76 Na2CO3·10H2O
Nesquehonite -3.61 -8.12 -4.51 MgCO3·3H2O
Nsutite -12.85 4.66 17.50 MnO2
O2(g) -47.52 39.44 86.96 O2
Periclase -10.12 12.49 22.61 MgO
Portlandite -10.94 12.74 23.68 Ca(OH)2
Pyrochroite -4.83 11.02 15.85 Mn(OH)2
Pyrolusite -12.49 30.74 43.22 MnO2
Rhodochrosite 0.98 -9.59 -10.57 MnCO3
Rutherfordine -8.16 -22.64 -14.48 UO2CO3
Schoepite -8.36 -2.03 6.33 UO2(OH)2·H2O
Semetal(am) -4.26 -11.45 -7.18 Se
Semetal(hex) -3.63 -11.45 -7.82 Se
SeO2 -16.98 -16.87 0.12 SeO2
SeO3 -56.85 -34.82 22.04 SeO3
Siderite -0.13 -10.26 -10.13 FeCO3
Thenardite -7.74 -7.36 0.38 Na2SO4
Thermonatrite -10.48 -9.78 0.71 Na2CO3·H2O
U3O8 -19.59 4.78 24.37 U3O8
U4O9 -26.37 -26.49 -0.13 U4O9
UO2(am) -13.23 -11.55 1.68 UO2
UO2(NO3)2 -42.08 -29.37 12.71 UO2(NO3)2
UO2(NO3)2·2H2O -34.39 -29.37 5.02 UO2(NO3)2·2H2O
UO2(NO3)2·3H2O -32.82 -29.37 3.45 UO2(NO3)2·3H2O
UO2(NO3)2·6H2O -31.27 -29.37 1.91 UO2(NO3)2·6H2O
UO2(OH)2(beta) -8.02 -2.03 6.00 UO2(OH)2
UO2SeO4·4H2O -34.59 -36.84 -2.25 UO2SeO4·4H2O
UO3 -10.27 -2.03 8.25 UO3

Uraninite -7.41 -11.55 -4.14 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 15. SAG1-3

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

Elements	Molality	Moles
Alkalinity	3.601e-03	3.601e-03
Ca	4.597e-03	4.597e-03
Cl	2.505e-03	2.505e-03
Fe(2)	1.990e-05	1.990e-05
Fe(3)	1.076e-06	1.076e-06
K	1.252e-04	1.252e-04
Mg	2.187e-03	2.187e-03
Mn	1.117e-04	1.117e-04
Mo	2.286e-07	2.286e-07
N(-3)	3.917e-05	3.917e-05
N(5)	1.430e-06	1.430e-06
Na	5.444e-03	5.444e-03
O(0)	1.377e-05	1.377e-05
S(6)	6.389e-03	6.389e-03
Se	1.648e-09	1.648e-09
U	1.851e-08	1.851e-08

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

pH = 7.650
pe = 1.900
Activity of water = 1.000
Ionic strength (mol/kgw) = 2.616e-02
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 3.748e-03
Total CO2 (mol/kg) = 3.748e-03
Temperature (°C) = 13.90
Electrical balance (eq) = 5.550e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.74
Iterations = 21 (265 overall)
Total H = 1.110177e+02
Total O = 5.554365e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	1.6782	0.0956
N(-3)/N(5)	5.8076	0.3308
O(-2)/O(0)	13.3738	0.7617

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	2.204e-07	1.883e-07	-6.657	-6.725	-0.068	(0)	
H+	2.605e-08	2.239e-08	-7.584	-7.650	-0.066	0.00	
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.03	
C(4)	3.748e-03						
HCO3-	3.420e-03	2.958e-03	-2.466	-2.529	-0.063	(0)	
H2CO3	1.718e-04	1.718e-04	-3.765	-3.765	0.000	(0)	
CaHCO3+	8.794e-05	7.633e-05	-4.056	-4.117	-0.062	(0)	
MgHCO3+	3.142e-05	2.693e-05	-4.503	-4.570	-0.067	(0)	
CaCO3	1.153e-05	1.153e-05	-4.938	-4.938	0.000	(0)	

NaHCO3	9.490e-06	9.490e-06	-5.023	-5.023	0.000	(0)
CO3-2	9.042e-06	4.932e-06	-5.044	-5.307	-0.263	(0)
MgCO3	3.223e-06	3.223e-06	-5.492	-5.492	0.000	(0)
MnHCO3+	2.775e-06	2.394e-06	-5.557	-5.621	-0.064	(0)
NaCO3-	6.718e-07	5.811e-07	-6.173	-6.236	-0.063	(0)
FeHCO3+	2.495e-07	2.166e-07	-6.603	-6.664	-0.062	(0)
Ca2UO2(CO3)3	1.418e-08	1.427e-08	-7.848	-7.846	0.003	(0)
CaUO2(CO3)3-2	4.172e-09	2.276e-09	-8.380	-8.643	-0.263	(0)
UO2(CO3)3-4	1.167e-10	5.901e-12	-9.933	-11.229	-1.296	(0)
UO2(CO3)2-2	2.102e-11	9.966e-12	-10.677	-11.001	-0.324	(0)
MgUO2(CO3)3-2	1.444e-11	7.878e-12	-10.840	-11.104	-0.263	(0)
UO2CO3	1.221e-13	1.221e-13	-12.913	-12.913	0.000	(0)
(UO2)2CO3(OH)3-	3.589e-18	3.084e-18	-17.445	-17.511	-0.066	(0)
(UO2)3(CO3)6-6	3.140e-27	1.343e-29	-26.503	-28.872	-2.369	(0)
Ca	4.597e-03					
Ca+2	3.471e-03	1.893e-03	-2.460	-2.723	-0.263	(0)
CaSO4	1.027e-03	1.027e-03	-2.989	-2.989	0.000	(0)
CaHCO3+	8.794e-05	7.633e-05	-4.056	-4.117	-0.062	(0)
CaCO3	1.153e-05	1.153e-05	-4.938	-4.938	0.000	(0)
Ca2UO2(CO3)3	1.418e-08	1.427e-08	-7.848	-7.846	0.003	(0)
CaNO3+	9.579e-09	7.949e-09	-8.019	-8.100	-0.081	(0)
CaOH+	7.199e-09	6.248e-09	-8.143	-8.204	-0.062	(0)
CaUO2(CO3)3-2	4.172e-09	2.276e-09	-8.380	-8.643	-0.263	(0)
CaNH3+2	4.099e-09	1.944e-09	-8.387	-8.711	-0.324	(0)
Ca(NH3)2+2	1.331e-15	6.311e-16	-14.876	-15.200	-0.324	(0)
Cl	2.505e-03					
Cl-	2.505e-03	2.153e-03	-2.601	-2.667	-0.066	(0)
MnCl+	1.356e-07	1.170e-07	-6.868	-6.932	-0.064	(0)
MnCl2	3.559e-10	3.559e-10	-9.449	-9.449	0.000	(0)
MnCl3-	2.445e-13	2.110e-13	-12.612	-12.676	-0.064	(0)
FeCl+2	1.361e-18	7.545e-19	-17.866	-18.122	-0.256	(0)
UO2Cl+	2.170e-20	1.801e-20	-19.664	-19.745	-0.081	(0)
FeCl2+	1.204e-20	1.039e-20	-19.919	-19.984	-0.064	(0)
UO2Cl2	2.285e-24	2.299e-24	-23.641	-23.638	0.003	(0)
FeCl3	2.236e-24	2.236e-24	-23.651	-23.651	0.000	(0)
UCl+3	0.000e+00	0.000e+00	-41.489	-42.218	-0.729	(0)
Fe(2)	1.990e-05					
Fe+2	1.540e-05	7.304e-06	-4.812	-5.136	-0.324	(0)
FeSO4	4.184e-06	4.184e-06	-5.378	-5.378	0.000	(0)
FeHCO3+	2.495e-07	2.166e-07	-6.603	-6.664	-0.062	(0)
FeOH+	6.345e-08	5.474e-08	-7.198	-7.262	-0.064	(0)
Fe(OH)2	7.226e-12	7.226e-12	-11.141	-11.141	0.000	(0)
Fe(OH)3-	1.071e-12	9.238e-13	-11.970	-12.034	-0.064	(0)
Fe(3)	1.076e-06					
Fe(OH)2+	9.753e-07	8.436e-07	-6.011	-6.074	-0.063	(0)
Fe(OH)3	8.068e-08	8.068e-08	-7.093	-7.093	0.000	(0)
Fe(OH)4-	1.972e-08	1.705e-08	-7.705	-7.768	-0.063	(0)
FeOH+2	4.533e-12	2.512e-12	-11.344	-11.600	-0.256	(0)
FeSO4+	3.867e-16	3.337e-16	-15.413	-15.477	-0.064	(0)
Fe+3	6.496e-17	1.661e-17	-16.187	-16.780	-0.592	(0)
Fe(SO4)2-	2.488e-17	2.065e-17	-16.604	-16.685	-0.081	(0)
FeCl+2	1.361e-18	7.545e-19	-17.866	-18.122	-0.256	(0)
FeCl2+	1.204e-20	1.039e-20	-19.919	-19.984	-0.064	(0)
Fe2(OH)2+4	6.201e-21	3.135e-22	-20.208	-21.504	-1.296	(0)
FeNO3+2	7.615e-22	3.611e-22	-21.118	-21.442	-0.324	(0)
FeHSeO3+2	6.659e-23	3.157e-23	-22.177	-22.501	-0.324	(0)
FeCl3	2.236e-24	2.236e-24	-23.651	-23.651	0.000	(0)
Fe3(OH)4+5	3.598e-25	3.394e-27	-24.444	-26.469	-2.025	(0)
H(0)	1.254e-22					
H2	6.270e-23	6.307e-23	-22.203	-22.200	0.003	(0)
K	1.252e-04					
K+	1.231e-04	1.058e-04	-3.910	-3.976	-0.066	(0)
KSO4-	2.147e-06	1.857e-06	-5.668	-5.731	-0.063	(0)
Mg	2.187e-03					
Mg+2	1.736e-03	9.472e-04	-2.760	-3.024	-0.263	(0)
MgSO4	4.163e-04	4.163e-04	-3.381	-3.381	0.000	(0)

MgHCO3+	3.142e-05	2.693e-05	-4.503	-4.570	-0.067	(0)
MgCO3	3.223e-06	3.223e-06	-5.492	-5.492	0.000	(0)
MgOH+	6.764e-08	5.887e-08	-7.170	-7.230	-0.060	(0)
MgUO2(CO3)3-2	1.444e-11	7.878e-12	-10.840	-11.104	-0.263	(0)
Mn(2)	1.117e-04					
Mn+2	9.106e-05	4.318e-05	-4.041	-4.365	-0.324	(0)
MnSO4	1.773e-05	1.773e-05	-4.751	-4.751	0.000	(0)
MnHCO3+	2.775e-06	2.394e-06	-5.557	-5.621	-0.064	(0)
MnCl+	1.356e-07	1.170e-07	-6.868	-6.932	-0.064	(0)
MnOH+	2.367e-08	2.042e-08	-7.626	-7.690	-0.064	(0)
MnCl2	3.559e-10	3.559e-10	-9.449	-9.449	0.000	(0)
MnNO3+	1.006e-10	8.352e-11	-9.997	-10.078	-0.081	(0)
MnCl3-	2.445e-13	2.110e-13	-12.612	-12.676	-0.064	(0)
Mn(NO3)2	2.627e-16	2.627e-16	-15.581	-15.581	0.000	(0)
Mn(OH)3-	7.061e-17	6.092e-17	-16.151	-16.215	-0.064	(0)
Mn(OH)4-2	1.596e-22	8.843e-23	-21.797	-22.053	-0.256	(0)
MnSeO4	1.190e-22	1.190e-22	-21.924	-21.924	0.000	(0)
MnSe	3.069e-24	3.069e-24	-23.513	-23.513	0.000	(0)
Mn(3)	1.115e-28					
Mn+3	1.115e-28	2.851e-29	-27.953	-28.545	-0.592	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-58.548	-58.804	-0.256	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-66.963	-67.032	-0.070	(0)
Mo	2.286e-07					
MoO4-2	2.285e-07	1.247e-07	-6.641	-6.904	-0.263	(0)
HMoO4-	4.898e-11	4.064e-11	-10.310	-10.391	-0.081	(0)
H2MoO4	1.366e-14	1.366e-14	-13.865	-13.865	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-52.078	-54.995	-2.916	(0)
HMo7O24-5	0.000e+00	0.000e+00	-54.301	-56.326	-2.025	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-57.918	-59.214	-1.296	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-62.875	-63.604	-0.729	(0)
N(-3)	3.917e-05					
NH4+	3.776e-05	3.202e-05	-4.423	-4.495	-0.072	(0)
NH4SO4-	1.051e-06	9.071e-07	-5.978	-6.042	-0.064	(0)
NH3	3.624e-07	3.624e-07	-6.441	-6.441	0.000	(0)
CaNH3+2	4.099e-09	1.944e-09	-8.387	-8.711	-0.324	(0)
Ca(NH3)2+2	1.331e-15	6.311e-16	-14.876	-15.200	-0.324	(0)
N(5)	1.430e-06					
NO3-	1.420e-06	1.220e-06	-5.848	-5.914	-0.066	(0)
CaNO3+	9.579e-09	7.949e-09	-8.019	-8.100	-0.081	(0)
MnNO3+	1.006e-10	8.352e-11	-9.997	-10.078	-0.081	(0)
Mn(NO3)2	2.627e-16	2.627e-16	-15.581	-15.581	0.000	(0)
FeNO3+2	7.615e-22	3.611e-22	-21.118	-21.442	-0.324	(0)
UO2NO3+	2.342e-23	1.944e-23	-22.630	-22.711	-0.081	(0)
Na	5.444e-03					
Na+	5.359e-03	4.606e-03	-2.271	-2.337	-0.066	(0)
NaSO4-	7.444e-05	6.438e-05	-4.128	-4.191	-0.063	(0)
NaHCO3	9.490e-06	9.490e-06	-5.023	-5.023	0.000	(0)
NaCO3-	6.718e-07	5.811e-07	-6.173	-6.236	-0.063	(0)
O(0)	1.377e-05					
O2	6.884e-06	6.925e-06	-5.162	-5.160	0.003	(0)
S(6)	6.389e-03					
SO4-2	4.847e-03	2.644e-03	-2.315	-2.578	-0.263	(0)
CaSO4	1.027e-03	1.027e-03	-2.989	-2.989	0.000	(0)
MgSO4	4.163e-04	4.163e-04	-3.381	-3.381	0.000	(0)
NaSO4-	7.444e-05	6.438e-05	-4.128	-4.191	-0.063	(0)
MnSO4	1.773e-05	1.773e-05	-4.751	-4.751	0.000	(0)
FeSO4	4.184e-06	4.184e-06	-5.378	-5.378	0.000	(0)
KSO4-	2.147e-06	1.857e-06	-5.668	-5.731	-0.063	(0)
NH4SO4-	1.051e-06	9.071e-07	-5.978	-6.042	-0.064	(0)
HSO4-	4.771e-09	4.104e-09	-8.321	-8.387	-0.065	(0)
FeSO4+	3.867e-16	3.337e-16	-15.413	-15.477	-0.064	(0)
Fe(SO4)2-	2.488e-17	2.065e-17	-16.604	-16.685	-0.081	(0)
UO2SO4	1.939e-17	1.939e-17	-16.712	-16.712	0.000	(0)
UO2(SO4)2-2	1.076e-18	5.104e-19	-17.968	-18.292	-0.324	(0)

U(SO4)2	5.424e-37	5.424e-37	-36.266	-36.266	0.000	(0)
USO4+2	8.044e-38	3.814e-38	-37.095	-37.419	-0.324	(0)
Se(-2)	4.685e-22					
HSe-	4.653e-22	3.861e-22	-21.332	-21.413	-0.081	(0)
MnSe	3.069e-24	3.069e-24	-23.513	-23.513	0.000	(0)
H2Se	6.374e-26	6.374e-26	-25.196	-25.196	0.000	(0)
Se-2	1.717e-29	8.143e-30	-28.765	-29.089	-0.324	(0)
Se(4)	1.648e-09					
HSeO3-	1.280e-09	1.062e-09	-8.893	-8.974	-0.081	(0)
SeO3-2	3.684e-10	1.747e-10	-9.434	-9.758	-0.324	(0)
H2SeO3	9.209e-15	9.209e-15	-14.036	-14.036	0.000	(0)
FeHSeO3+2	6.659e-23	3.157e-23	-22.177	-22.501	-0.324	(0)
Se(6)	2.347e-20					
SeO4-2	2.335e-20	1.274e-20	-19.632	-19.895	-0.263	(0)
MnSeO4	1.190e-22	1.190e-22	-21.924	-21.924	0.000	(0)
HSeO4-	1.203e-26	9.983e-27	-25.920	-26.001	-0.081	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-52.045	-52.774	-0.729	(0)
U(4)	1.102e-17					
U(OH)5-	1.101e-17	9.139e-18	-16.958	-17.039	-0.081	(0)
U(OH)4	1.030e-20	1.030e-20	-19.987	-19.987	0.000	(0)
U(OH)3+	1.167e-24	9.682e-25	-23.933	-24.014	-0.081	(0)
U(OH)2+2	2.914e-29	1.382e-29	-28.535	-28.860	-0.324	(0)
UOH+3	1.179e-34	2.199e-35	-33.929	-34.658	-0.729	(0)
U(SO4)2	5.424e-37	5.424e-37	-36.266	-36.266	0.000	(0)
USO4+2	8.044e-38	3.814e-38	-37.095	-37.419	-0.324	(0)
U+4	0.000e+00	0.000e+00	-40.090	-41.387	-1.296	(0)
UCl+3	0.000e+00	0.000e+00	-41.489	-42.218	-0.729	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-144.166	-150.727	-6.562	(0)
U(5)	7.591e-17					
UO2+	7.591e-17	6.300e-17	-16.120	-16.201	-0.081	(0)
U(6)	1.851e-08					
Ca2UO2(CO3)3	1.418e-08	1.427e-08	-7.848	-7.846	0.003	(0)
CaUO2(CO3)3-2	4.172e-09	2.276e-09	-8.380	-8.643	-0.263	(0)
UO2(CO3)3-4	1.167e-10	5.901e-12	-9.933	-11.229	-1.296	(0)
UO2(CO3)2-2	2.102e-11	9.966e-12	-10.677	-11.001	-0.324	(0)
MgUO2(CO3)3-2	1.444e-11	7.878e-12	-10.840	-11.104	-0.263	(0)
UO2(OH)2	6.357e-13	6.396e-13	-12.197	-12.194	0.003	(0)
UO2CO3	1.221e-13	1.221e-13	-12.913	-12.913	0.000	(0)
UO2(OH)3-	4.114e-14	3.536e-14	-13.386	-13.451	-0.066	(0)
UO2OH+	2.142e-16	1.777e-16	-15.669	-15.750	-0.081	(0)
UO2SO4	1.939e-17	1.939e-17	-16.712	-16.712	0.000	(0)
UO2+2	1.213e-17	6.619e-18	-16.916	-17.179	-0.263	(0)
(UO2)2CO3(OH)3-	3.589e-18	3.084e-18	-17.445	-17.511	-0.066	(0)
UO2(SO4)2-2	1.076e-18	5.104e-19	-17.968	-18.292	-0.324	(0)
UO2(OH)4-2	4.511e-20	2.461e-20	-19.346	-19.609	-0.263	(0)
UO2Cl+	2.170e-20	1.801e-20	-19.664	-19.745	-0.081	(0)
UO2NO3+	2.342e-23	1.944e-23	-22.630	-22.711	-0.081	(0)
UO2Cl2	2.285e-24	2.299e-24	-23.641	-23.638	0.003	(0)
(UO2)2(OH)2+2	2.559e-25	1.213e-25	-24.592	-24.916	-0.324	(0)
(UO2)3(CO3)6-6	3.140e-27	1.343e-29	-26.503	-28.872	-2.369	(0)
(UO2)2OH+3	1.501e-29	3.839e-30	-28.824	-29.416	-0.592	(0)
(UO2)3(OH)7-	1.062e-29	9.130e-30	-28.974	-29.040	-0.066	(0)
(UO2)3(OH)5+	2.990e-30	2.481e-30	-29.524	-29.605	-0.081	(0)
(UO2)3(OH)4+2	2.489e-33	1.358e-33	-32.604	-32.867	-0.263	(0)
(UO2)4(OH)7+	8.853e-38	7.608e-38	-37.053	-37.119	-0.066	(0)

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

Phase SI** log IAP log K(287 K, 1 atm)

(NH4)2SeO4	-29.33	-28.88	0.45	(NH4)2SeO4
Anhydrite	-0.99	-5.30	-4.31	CaSO4
Aragonite	0.19	-8.03	-8.22	CaCO3
Artinite	-6.47	3.95	10.41	MgCO3:Mg(OH)2:3H2O
Birnessite	-14.14	3.95	18.09	MnO2

Bixbyite	-11.39	-11.19	0.20	Mn2O3
Brucite	-5.34	12.28	17.62	Mg(OH)2
Calcite	0.40	-8.03	-8.43	CaCO3
CaMoO4	-1.69	-9.63	-7.94	CaMoO4
CaSeO3:2H2O	-6.99	-4.05	2.95	CaSeO3:2H2O
CaSeO4:2H2O	-19.65	-22.62	-2.96	CaSeO4:2H2O
CH4(g)	-54.22	-97.01	-42.79	CH4
CO2(g)	-2.43	-20.61	-18.17	CO2
Dolomite(disordered)	-0.13	-16.36	-16.23	CaMg(CO3)2
Dolomite(ordered)	0.46	-16.36	-16.82	CaMg(CO3)2
Epsomite	-3.40	-5.60	-2.20	MgSO4:7H2O
Fe(OH)2	-3.40	10.16	13.56	Fe(OH)2
Fe(OH)2.7Cl.3	6.11	3.07	-3.04	Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-5.84	-4.28	1.55	Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-16.90	-37.53	-20.63	Fe2(SeO3)3:2H2O
Fe2(SO4)3	-39.20	-41.29	-2.09	Fe2(SO4)3
Fe3(OH)8	2.28	22.50	20.22	Fe3(OH)8
FeMoO4	-2.02	-12.04	-10.02	FeMoO4
Ferrihydrite	2.48	6.17	3.69	Fe(OH)3
Ferroselite	-9.95	-28.86	-18.92	FeSe2
FeSe	-7.89	-18.90	-11.01	FeSe
Goethite	5.27	6.17	0.90	FeOOH
Gummite	-10.10	-1.88	8.22	UO3
Gypsum	-0.68	-5.30	-4.62	CaSO4:2H2O
H-Jarosite	-6.71	-17.25	-10.54	(H3O)Fe3(SO4)2(OH)6
H2MoO4	-9.00	-22.20	-13.21	H2MoO4
H2Se(g)	-24.21	-29.06	-4.86	H2Se
Halite	-6.58	-5.00	1.58	NaCl
Hausmannite	-11.98	51.91	63.88	Mn3O4
Hematite	12.88	12.34	-0.54	Fe2O3
Huntite	-3.78	-33.02	-29.24	CaMg3(CO3)4
Hydromagnesite	-13.76	-21.05	-7.29	Mg5(CO3)4(OH)2:4H2O
K-Jarosite	0.34	-13.57	-13.91	KFe3(SO4)2(OH)6
K2MoO4	-18.14	-14.86	3.28	K2MoO4
K2SeO4	-27.12	-27.85	-0.73	K2SeO4
Lepidocrocite	4.80	6.17	1.37	FeOOH
Lime	-21.44	12.58	34.01	CaO
Maghemite	5.95	12.34	6.39	Fe2O3
Magnesioferrite	5.87	24.62	18.75	Fe2MgO4
Magnesite	-0.74	-8.33	-7.60	MgCO3
Magnetite	17.69	22.50	4.82	Fe3O4
Manganite	-4.86	20.48	25.34	MnOOH
Melanterite	-5.37	-7.72	-2.35	FeSO4:7H2O
Mg(OH)2(active)	-6.52	12.28	18.79	Mg(OH)2
MgMoO4	-8.08	-9.93	-1.85	MgMoO4
MgSeO3:6H2O	-7.37	-4.35	3.02	MgSeO3:6H2O
MgSeO4:6H2O	-21.72	-22.92	-1.20	MgSeO4:6H2O
Mirabilite	-5.60	-7.25	-1.65	Na2SO4:10H2O
Mn2(SO4)3	-60.22	-64.82	-4.60	Mn2(SO4)3
MnCl2:4H2O	-12.49	-9.70	2.79	MnCl2:4H2O
MnSe	-22.29	-18.13	4.16	MnSe
MnSeO3	-6.82	-5.69	1.13	MnSeO3
MnSeO3:2H2O	-6.61	-5.69	0.92	MnSeO3:2H2O
MnSeO4:5H2O	-22.21	-24.26	-2.05	MnSeO4:5H2O
MnSO4	-9.96	-6.94	3.02	MnSO4
MoO3	-14.20	-22.20	-8.00	MoO3
Na-Jarosite	-1.76	-11.93	-10.17	NaFe3(SO4)2(OH)6
Na2Mo2O7	-16.80	-33.78	-16.98	Na2Mo2O7
Na2MoO4	-13.14	-11.58	1.56	Na2MoO4
Na2MoO4:2H2O	-12.80	-11.58	1.22	Na2MoO4:2H2O
Na2SeO3:5H2O	-16.30	-6.00	10.30	Na2SeO3:5H2O
Na2SeO4	-25.85	-24.57	1.28	Na2SeO4
Natron	-8.22	-9.98	-1.76	Na2CO3:10H2O
Nesquehonite	-3.83	-8.33	-4.51	MgCO3:3H2O
Nsutite	-13.55	3.95	17.50	MnO2
O2(g)	-48.76	38.20	86.96	O2

Periclase -10.33 12.28 22.61 MgO
 Portlandite -11.10 12.58 23.68 Ca(OH)2
 Pyrochroite -4.92 10.93 15.85 Mn(OH)2
 Pyrolusite -13.19 30.03 43.22 MnO2
 Rhodochrosite 0.90 -9.67 -10.57 MnCO3
 Rutherfordine -8.01 -22.49 -14.48 UO2CO3
 Schoepite -8.21 -1.88 6.33 UO2(OH)2:H2O
 Semetal(am) -2.78 -9.96 -7.18 Se
 Semetal(hex) -2.15 -9.96 -7.82 Se
 SeO2 -16.74 -16.62 0.12 SeO2
 SeO3 -57.23 -35.19 22.04 SeO3
 Siderite -0.31 -10.44 -10.13 FeCO3
 Thenardite -7.63 -7.25 0.38 Na2SO4
 Thermonatrite -10.69 -9.98 0.71 Na2CO3:H2O
 U3O8 -18.53 5.84 24.37 U3O8
 U4O9 -23.92 -24.05 -0.13 U4O9
 UO2(am) -12.46 -10.79 1.68 UO2
 UO2(NO3)2 -41.72 -29.01 12.71 UO2(NO3)2
 UO2(NO3)2:2H2O -34.03 -29.01 5.02 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -32.46 -29.01 3.45 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -30.91 -29.01 1.91 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -7.88 -1.88 6.00 UO2(OH)2
 UO2SeO4:4H2O -34.82 -37.07 -2.25 UO2SeO4:4H2O
 UO3 -10.13 -1.88 8.25 UO3
 Uraninite -6.65 -10.79 -4.14 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 16. SAG1-4

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

Elements	Molality	Moles
Alkalinity	2.982e-03	2.982e-03
Ca	8.623e-03	8.623e-03
Cl	9.861e-04	9.861e-04
Fe(2)	3.964e-05	3.964e-05
Fe(3)	2.242e-05	2.242e-05
K	9.505e-05	9.505e-05
Mg	2.629e-03	2.629e-03
Mn	3.665e-05	3.665e-05
Mo	6.473e-08	6.473e-08
N(-3)	7.795e-06	7.795e-06
N(5)	1.430e-06	1.430e-06
Na	3.342e-03	3.342e-03
O(0)	1.315e-05	1.315e-05
S(6)	1.084e-02	1.084e-02
Se	1.269e-09	1.269e-09
U	5.808e-09	5.808e-09

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

pH = 7.530
 pe = 1.300
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 3.519e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.142e-03
 Total CO2 (mol/kg) = 3.142e-03
 Temperature (°C) = 13.90
 Electrical balance (eq) = 4.657e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.20
 Iterations = 10 (275 overall)
 Total H = 1.110170e+02

Total O = 5.555970e+01

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

Redox couple	pe Eh (volts)	
Fe(2)/Fe(3)	3.0191	0.1719
N(-3)/N(5)	6.0458	0.3443
O(-2)/O(0)	13.4890	0.7682

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.706e-07	1.428e-07	-6.768	-6.845	-0.077	(0)	
H+	3.498e-08	2.951e-08	-7.456	-7.530	-0.074	0.00	
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.03	
C(4)	3.142e-03						
HCO3-	2.792e-03	2.374e-03	-2.554	-2.625	-0.071	(0)	
H2CO3	1.817e-04	1.817e-04	-3.741	-3.741	0.000	(0)	
CaHCO3+	1.162e-04	9.919e-05	-3.935	-4.004	-0.069	(0)	
MgHCO3+	2.695e-05	2.265e-05	-4.569	-4.645	-0.075	(0)	
CaCO3	1.137e-05	1.137e-05	-4.944	-4.944	0.000	(0)	
CO3-2	5.926e-06	3.003e-06	-5.227	-5.523	-0.295	(0)	
NaHCO3	4.563e-06	4.563e-06	-5.341	-5.341	0.000	(0)	
MgCO3	2.056e-06	2.056e-06	-5.687	-5.687	0.000	(0)	
MnHCO3+	6.344e-07	5.376e-07	-6.198	-6.270	-0.072	(0)	
FeHCO3+	3.397e-07	2.900e-07	-6.469	-6.538	-0.069	(0)	
NaCO3-	2.493e-07	2.119e-07	-6.603	-6.674	-0.071	(0)	
Ca2UO2(CO3)3	4.829e-09	4.869e-09	-8.316	-8.313	0.004	(0)	
CaUO2(CO3)3-2	9.465e-10	4.795e-10	-9.024	-9.319	-0.295	(0)	
UO2(CO3)3-4	2.446e-11	7.678e-13	-10.612	-12.115	-1.503	(0)	
UO2(CO3)2-2	5.060e-12	2.130e-12	-11.296	-11.672	-0.376	(0)	
MgUO2(CO3)3-2	2.120e-12	1.074e-12	-11.674	-11.969	-0.295	(0)	
UO2CO3	4.287e-14	4.287e-14	-13.368	-13.368	0.000	(0)	
(UO2)2CO3(OH)3-	3.230e-19	2.725e-19	-18.491	-18.565	-0.074	(0)	
(UO2)3(CO3)6-6	5.959e-29	1.311e-31	-28.225	-30.882	-2.658	(0)	
Ca	8.623e-03						
Ca+2	6.051e-03	3.066e-03	-2.218	-2.513	-0.295	(0)	
CaSO4	2.444e-03	2.444e-03	-2.612	-2.612	0.000	(0)	
CaHCO3+	1.162e-04	9.919e-05	-3.935	-4.004	-0.069	(0)	
CaCO3	1.137e-05	1.137e-05	-4.944	-4.944	0.000	(0)	
CaNO3+	1.563e-08	1.259e-08	-7.806	-7.900	-0.094	(0)	
CaOH+	8.990e-09	7.675e-09	-8.046	-8.115	-0.069	(0)	
Ca2UO2(CO3)3	4.829e-09	4.869e-09	-8.316	-8.313	0.004	(0)	
CaNH3+2	1.092e-09	4.598e-10	-8.962	-9.337	-0.376	(0)	
CaUO2(CO3)3-2	9.465e-10	4.795e-10	-9.024	-9.319	-0.295	(0)	
Ca(NH3)2+2	5.181e-17	2.181e-17	-16.286	-16.661	-0.376	(0)	
Cl	9.861e-04						
Cl-	9.861e-04	8.319e-04	-3.006	-3.080	-0.074	(0)	
MnCl+	1.493e-08	1.265e-08	-7.826	-7.898	-0.072	(0)	
MnCl2	1.487e-11	1.487e-11	-10.828	-10.828	0.000	(0)	
MnCl3-	4.021e-15	3.407e-15	-14.396	-14.468	-0.072	(0)	
FeCl+2	2.069e-17	1.067e-17	-16.684	-16.972	-0.288	(0)	
FeCl2+	6.696e-20	5.674e-20	-19.174	-19.246	-0.072	(0)	
UO2Cl+	4.982e-21	4.013e-21	-20.303	-20.397	-0.094	(0)	
FeCl3	4.721e-24	4.721e-24	-23.326	-23.326	0.000	(0)	
UO2Cl2	1.964e-25	1.980e-25	-24.707	-24.703	0.004	(0)	
UCl+3	0.000e+00	0.000e+00	-40.345	-41.190	-0.846	(0)	
Fe(2)	3.964e-05						
Fe+2	2.895e-05	1.219e-05	-4.538	-4.914	-0.376	(0)	
FeSO4	1.027e-05	1.027e-05	-4.989	-4.989	0.000	(0)	
FeHCO3+	3.397e-07	2.900e-07	-6.469	-6.538	-0.069	(0)	
FeOH+	8.176e-08	6.929e-08	-7.087	-7.159	-0.072	(0)	
Fe(OH)2	6.937e-12	6.937e-12	-11.159	-11.159	0.000	(0)	

Fe(OH)3- 7.939e-13 6.728e-13 -12.100 -12.172 -0.072 (0)
 Fe(3) 2.242e-05
 Fe(OH)2+ 2.089e-05 1.776e-05 -4.680 -4.751 -0.071 (0)
 Fe(OH)3 1.288e-06 1.288e-06 -5.890 -5.890 0.000 (0)
 Fe(OH)4- 2.430e-07 2.065e-07 -6.614 -6.685 -0.071 (0)
 FeOH+2 1.352e-10 6.971e-11 -9.869 -10.157 -0.288 (0)
 FeSO4+ 2.118e-14 1.795e-14 -13.674 -13.746 -0.072 (0)
 Fe+3 2.806e-15 6.078e-16 -14.552 -15.216 -0.664 (0)
 Fe(SO4)2- 2.027e-15 1.633e-15 -14.693 -14.787 -0.094 (0)
 FeCl+2 2.069e-17 1.067e-17 -16.684 -16.972 -0.288 (0)
 Fe2(OH)2+4 7.689e-18 2.414e-19 -17.114 -18.617 -1.503 (0)
 FeCl2+ 6.696e-20 5.674e-20 -19.174 -19.246 -0.072 (0)
 FeNO3+2 3.069e-20 1.292e-20 -19.513 -19.889 -0.376 (0)
 Fe3(OH)4+5 1.228e-20 5.502e-23 -19.911 -22.260 -2.349 (0)
 FeHSeO3+2 2.131e-21 8.970e-22 -20.671 -21.047 -0.376 (0)
 FeCl3 4.721e-24 4.721e-24 -23.326 -23.326 0.000 (0)
 H(0) 3.446e-21
 H2 1.723e-21 1.737e-21 -20.764 -20.760 0.004 (0)
 K 9.505e-05
 K+ 9.268e-05 7.819e-05 -4.033 -4.107 -0.074 (0)
 KSO4- 2.375e-06 2.018e-06 -5.624 -5.695 -0.071 (0)
 Mg 2.629e-03
 Mg+2 1.959e-03 9.926e-04 -2.708 -3.003 -0.295 (0)
 MgSO4 6.414e-04 6.414e-04 -3.193 -3.193 0.000 (0)
 MgHCO3+ 2.695e-05 2.265e-05 -4.569 -4.645 -0.075 (0)
 MgCO3 2.056e-06 2.056e-06 -5.687 -5.687 0.000 (0)
 MgOH+ 5.462e-08 4.680e-08 -7.263 -7.330 -0.067 (0)
 MgUO2(CO3)3-2 2.120e-12 1.074e-12 -11.674 -11.969 -0.295 (0)
 Mn(2) 3.665e-05
 Mn+2 2.870e-05 1.208e-05 -4.542 -4.918 -0.376 (0)
 MnSO4 7.292e-06 7.292e-06 -5.137 -5.137 0.000 (0)
 MnHCO3+ 6.344e-07 5.376e-07 -6.198 -6.270 -0.072 (0)
 MnCl+ 1.493e-08 1.265e-08 -7.826 -7.898 -0.072 (0)
 MnOH+ 5.114e-09 4.334e-09 -8.291 -8.363 -0.072 (0)
 MnNO3+ 2.837e-11 2.286e-11 -10.547 -10.641 -0.094 (0)
 MnCl2 1.487e-11 1.487e-11 -10.828 -10.828 0.000 (0)
 MnCl3- 4.021e-15 3.407e-15 -14.396 -14.468 -0.072 (0)
 Mn(NO3)2 7.032e-17 7.032e-17 -16.153 -16.153 0.000 (0)
 Mn(OH)3- 8.779e-18 7.440e-18 -17.057 -17.128 -0.072 (0)
 MnSe 1.057e-20 1.057e-20 -19.976 -19.976 0.000 (0)
 Mn(OH)4-2 1.589e-23 8.192e-24 -22.799 -23.087 -0.288 (0)
 MnSeO4 7.121e-25 7.121e-25 -24.147 -24.147 0.000 (0)
 Mn(3) 9.252e-30
 Mn+3 9.252e-30 2.004e-30 -29.034 -29.698 -0.664 (0)
 Mn(6) 0.000e+00
 MnO4-2 0.000e+00 0.000e+00 -62.430 -62.718 -0.288 (0)
 Mn(7) 0.000e+00
 MnO4- 0.000e+00 0.000e+00 -71.466 -71.546 -0.079 (0)
 Mo 6.473e-08
 MoO4-2 6.472e-08 3.279e-08 -7.189 -7.484 -0.295 (0)
 HMoO4- 1.750e-11 1.409e-11 -10.757 -10.851 -0.094 (0)
 H2MoO4 6.244e-15 6.244e-15 -14.205 -14.205 0.000 (0)
 Mo7O24-6 0.000e+00 0.000e+00 -54.712 -58.094 -3.382 (0)
 HMo7O24-5 0.000e+00 0.000e+00 -56.957 -59.305 -2.349 (0)
 H2Mo7O24-4 0.000e+00 0.000e+00 -60.570 -62.074 -1.503 (0)
 H3Mo7O24-3 0.000e+00 0.000e+00 -65.498 -66.344 -0.846 (0)
 N(-3) 7.795e-06
 NH4+ 7.438e-06 6.166e-06 -5.129 -5.210 -0.081 (0)
 NH4SO4- 3.031e-07 2.568e-07 -6.518 -6.590 -0.072 (0)
 NH3 5.293e-08 5.293e-08 -7.276 -7.276 0.000 (0)
 CaNH3+2 1.092e-09 4.598e-10 -8.962 -9.337 -0.376 (0)
 Ca(NH3)2+2 5.181e-17 2.181e-17 -16.286 -16.661 -0.376 (0)
 N(5) 1.430e-06
 NO3- 1.415e-06 1.194e-06 -5.849 -5.923 -0.074 (0)
 CaNO3+ 1.563e-08 1.259e-08 -7.806 -7.900 -0.094 (0)
 MnNO3+ 2.837e-11 2.286e-11 -10.547 -10.641 -0.094 (0)

Mn(NO3)2	7.032e-17	7.032e-17	-16.153	-16.153	0.000	(0)
FeNO3+2	3.069e-20	1.292e-20	-19.513	-19.889	-0.376	(0)
UO2NO3+	1.361e-23	1.096e-23	-22.866	-22.960	-0.094	(0)
Na	3.342e-03					
Na+	3.270e-03	2.759e-03	-2.485	-2.559	-0.074	(0)
NaSO4-	6.672e-05	5.671e-05	-4.176	-4.246	-0.071	(0)
NaHCO3	4.563e-06	4.563e-06	-5.341	-5.341	0.000	(0)
NaCO3-	2.493e-07	2.119e-07	-6.603	-6.674	-0.071	(0)
O(0)	1.315e-05					
O2	6.574e-06	6.627e-06	-5.182	-5.179	0.004	(0)
S(6)	1.084e-02					
SO4-2	7.672e-03	3.887e-03	-2.115	-2.410	-0.295	(0)
CaSO4	2.444e-03	2.444e-03	-2.612	-2.612	0.000	(0)
MgSO4	6.414e-04	6.414e-04	-3.193	-3.193	0.000	(0)
NaSO4-	6.672e-05	5.671e-05	-4.176	-4.246	-0.071	(0)
FeSO4	1.027e-05	1.027e-05	-4.989	-4.989	0.000	(0)
MnSO4	7.292e-06	7.292e-06	-5.137	-5.137	0.000	(0)
KSO4-	2.375e-06	2.018e-06	-5.624	-5.695	-0.071	(0)
NH4SO4-	3.031e-07	2.568e-07	-6.518	-6.590	-0.072	(0)
HSO4-	9.424e-09	7.954e-09	-8.026	-8.099	-0.074	(0)
FeSO4+	2.118e-14	1.795e-14	-13.674	-13.746	-0.072	(0)
Fe(SO4)2-	2.027e-15	1.633e-15	-14.693	-14.787	-0.094	(0)
UO2SO4	1.644e-17	1.644e-17	-16.784	-16.784	0.000	(0)
UO2(SO4)2-2	1.511e-18	6.362e-19	-17.821	-18.196	-0.376	(0)
U(SO4)2	3.236e-35	3.236e-35	-34.490	-34.490	0.000	(0)
USO4+2	3.678e-36	1.548e-36	-35.434	-35.810	-0.376	(0)
Se(-2)	7.792e-18					
HSe-	7.780e-18	6.266e-18	-17.109	-17.203	-0.094	(0)
MnSe	1.057e-20	1.057e-20	-19.976	-19.976	0.000	(0)
H2Se	1.364e-21	1.364e-21	-20.865	-20.865	0.000	(0)
Se-2	2.381e-25	1.002e-25	-24.623	-24.999	-0.376	(0)
Se(4)	1.269e-09					
HSeO3-	1.024e-09	8.250e-10	-8.990	-9.084	-0.094	(0)
SeO3-2	2.445e-10	1.029e-10	-9.612	-9.988	-0.376	(0)
H2SeO3	9.428e-15	9.428e-15	-14.026	-14.026	0.000	(0)
FeHSeO3+2	2.131e-21	8.970e-22	-20.671	-21.047	-0.376	(0)
Se(6)	5.384e-22					
SeO4-2	5.377e-22	2.724e-22	-21.269	-21.565	-0.295	(0)
MnSeO4	7.121e-25	7.121e-25	-24.147	-24.147	0.000	(0)
HSeO4-	3.494e-28	2.815e-28	-27.457	-27.551	-0.094	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-49.888	-50.733	-0.846	(0)
U(4)	7.875e-17					
U(OH)5-	7.865e-17	6.335e-17	-16.104	-16.198	-0.094	(0)
U(OH)4	9.414e-20	9.414e-20	-19.026	-19.026	0.000	(0)
U(OH)3+	1.448e-23	1.167e-23	-22.839	-22.933	-0.094	(0)
U(OH)2+2	5.214e-28	2.195e-28	-27.283	-27.659	-0.376	(0)
UOH+3	3.227e-33	4.605e-34	-32.491	-33.337	-0.846	(0)
U(SO4)2	3.236e-35	3.236e-35	-34.490	-34.490	0.000	(0)
USO4+2	3.678e-36	1.548e-36	-35.434	-35.810	-0.376	(0)
U+4	3.610e-39	1.133e-40	-38.443	-39.946	-1.503	(0)
UCI+3	0.000e+00	0.000e+00	-40.345	-41.190	-0.846	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-136.272	-143.882	-7.610	(0)
U(5)	1.796e-16					
UO2+	1.796e-16	1.446e-16	-15.746	-15.840	-0.094	(0)
U(6)	5.808e-09					
Ca2UO2(CO3)3	4.829e-09	4.869e-09	-8.316	-8.313	0.004	(0)
CaUO2(CO3)3-2	9.465e-10	4.795e-10	-9.024	-9.319	-0.295	(0)
UO2(CO3)3-4	2.446e-11	7.678e-13	-10.612	-12.115	-1.503	(0)
UO2(CO3)2-2	5.060e-12	2.130e-12	-11.296	-11.672	-0.376	(0)
MgUO2(CO3)3-2	2.120e-12	1.074e-12	-11.674	-11.969	-0.295	(0)
UO2(OH)2	2.105e-13	2.122e-13	-12.677	-12.673	0.004	(0)
UO2CO3	4.287e-14	4.287e-14	-13.368	-13.368	0.000	(0)
UO2(OH)3-	1.055e-14	8.900e-15	-13.977	-14.051	-0.074	(0)
UO2OH+	9.652e-17	7.775e-17	-16.015	-16.109	-0.094	(0)
UO2SO4	1.644e-17	1.644e-17	-16.784	-16.784	0.000	(0)

UO2+2 7.534e-18 3.817e-18 -17.123 -17.418 -0.295 (0)
 UO2(SO4)2-2 1.511e-18 6.362e-19 -17.821 -18.196 -0.376 (0)
 (UO2)2CO3(OH)3- 3.230e-19 2.725e-19 -18.491 -18.565 -0.074 (0)
 UO2(OH)4-2 9.272e-21 4.698e-21 -20.033 -20.328 -0.295 (0)
 UO2Cl+ 4.982e-21 4.013e-21 -20.303 -20.397 -0.094 (0)
 UO2NO3+ 1.361e-23 1.096e-23 -22.866 -22.960 -0.094 (0)
 UO2Cl2 1.964e-25 1.980e-25 -24.707 -24.703 0.004 (0)
 (UO2)2(OH)2+2 5.516e-26 2.322e-26 -25.258 -25.634 -0.376 (0)
 (UO2)3(CO3)6-6 5.959e-29 1.311e-31 -28.225 -30.882 -2.658 (0)
 (UO2)2OH+3 4.472e-30 9.686e-31 -29.349 -30.014 -0.664 (0)
 (UO2)3(OH)7- 2.999e-31 2.530e-31 -30.523 -30.597 -0.074 (0)
 (UO2)3(OH)5+ 1.483e-31 1.195e-31 -30.829 -30.923 -0.094 (0)
 (UO2)3(OH)4+2 1.701e-34 8.620e-35 -33.769 -34.064 -0.295 (0)
 (UO2)4(OH)7+ 1.441e-39 1.216e-39 -38.841 -38.915 -0.074 (0)

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

Phase	SI**	log IAP	log K(287 K, 1 atm)
(NH4)2SeO4	-32.43	-31.98	0.45 (NH4)2SeO4
Anhydrite	-0.61	-4.92	-4.31 CaSO4
Aragonite	0.18	-8.04	-8.22 CaCO3
Artinite	-6.88	3.53	10.41 MgCO3:Mg(OH)2:3H2O
Birnessite	-16.37	1.72	18.09 MnO2
Bixbyite	-14.42	-14.22	0.20 Mn2O3
Brucite	-5.56	12.06	17.62 Mg(OH)2
Calcite	0.39	-8.04	-8.43 CaCO3
CaMoO4	-2.06	-10.00	-7.94 CaMoO4
CaSeO3:2H2O	-7.01	-4.07	2.95 CaSeO3:2H2O
CaSeO4:2H2O	-21.11	-24.08	-2.96 CaSeO4:2H2O
CH4(g)	-48.43	-91.22	-42.79 CH4
CO2(g)	-2.41	-20.58	-18.17 CO2
Dolomite(disordered)	-0.34	-16.56	-16.23 CaMg(CO3)2
Dolomite(ordered)	0.26	-16.56	-16.82 CaMg(CO3)2
Epsomite	-3.21	-5.41	-2.20 MgSO4:7H2O
Fe(OH)2	-3.42	10.15	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	7.23	4.19	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-3.42	-1.87	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-14.47	-35.09	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-35.57	-37.66	-2.09 Fe2(SO4)3
Fe3(OH)8	4.67	24.89	20.22 Fe3(OH)8
FeMoO4	-2.38	-12.40	-10.02 FeMoO4
Ferrihydrite	3.69	7.37	3.69 Fe(OH)3
Ferroselite	-2.74	-21.66	-18.92 FeSe2
FeSe	-3.57	-14.59	-11.01 FeSe
Goethite	6.47	7.37	0.90 FeOOH
Gummite	-10.58	-2.36	8.22 UO3
Gypsum	-0.31	-4.92	-4.62 CaSO4:2H2O
H-Jarosite	-2.28	-12.82	-10.54 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-9.34	-22.54	-13.21 H2MoO4
H2Se(g)	-19.88	-24.73	-4.86 H2Se
Halite	-7.22	-5.64	1.58 NaCl
Hausmannite	-15.80	48.09	63.88 Mn3O4
Hematite	15.29	14.75	-0.54 Fe2O3
Huntite	-4.38	-33.61	-29.24 CaMg3(CO3)4
Hydromagnesite	-14.76	-22.05	-7.29 Mg5(CO3)4(OH)2:4H2O
K-Jarosite	4.52	-9.40	-13.91 KFe3(SO4)2(OH)6
K2MoO4	-18.98	-15.70	3.28 K2MoO4
K2SeO4	-29.05	-29.78	-0.73 K2SeO4
Lepidocrocite	6.00	7.37	1.37 FeOOH
Lime	-21.47	12.55	34.01 CaO
Maghemite	8.36	14.75	6.39 Fe2O3
Magnesioferrite	8.05	26.80	18.75 Fe2MgO4
Magnesite	-0.93	-8.53	-7.60 MgCO3
Magnetite	20.08	24.89	4.82 Fe3O4
Manganite	-6.37	18.97	25.34 MnOOH

Melanterite -4.98 -7.33 -2.35 FeSO4:7H2O
 Mg(OH)2(active) -6.74 12.06 18.79 Mg(OH)2
 MgMoO4 -8.64 -10.49 -1.85 MgMoO4
 MgSeO3:6H2O -7.58 -4.56 3.02 MgSeO3:6H2O
 MgSeO4:6H2O -23.37 -24.57 -1.20 MgSeO4:6H2O
 Mirabilite -5.88 -7.53 -1.65 Na2SO4:10H2O
 Mn2(SO4)3 -62.02 -66.63 -4.60 Mn2(SO4)3
 MnCl2:4H2O -13.87 -11.08 2.79 MnCl2:4H2O
 MnSe -18.76 -14.59 4.16 MnSe
 MnSeO3 -7.60 -6.47 1.13 MnSeO3
 MnSeO3:2H2O -7.40 -6.47 0.92 MnSeO3:2H2O
 MnSeO4:5H2O -24.43 -26.48 -2.05 MnSeO4:5H2O
 MnSO4 -10.35 -7.33 3.02 MnSO4
 MoO3 -14.54 -22.54 -8.00 MoO3
 Na-Jarosite 2.32 -7.85 -10.17 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -18.17 -35.15 -16.98 Na2Mo2O7
 Na2MoO4 -14.16 -12.60 1.56 Na2MoO4
 Na2MoO4:2H2O -13.83 -12.60 1.22 Na2MoO4:2H2O
 Na2SeO3:5H2O -16.97 -6.67 10.30 Na2SeO3:5H2O
 Na2SeO4 -27.96 -26.68 1.28 Na2SeO4
 Natron -8.89 -10.64 -1.76 Na2CO3:10H2O
 Nesquehonite -4.02 -8.53 -4.51 MgCO3:3H2O
 Nsutite -15.78 1.72 17.50 MnO2
 O2(g) -51.64 35.32 86.96 O2
 Periclase -10.55 12.06 22.61 MgO
 Portlandite -11.13 12.55 23.68 Ca(OH)2
 Pyrochroite -5.71 10.14 15.85 Mn(OH)2
 Pyrolusite -15.42 27.80 43.22 MnO2
 Rhodochrosite 0.13 -10.44 -10.57 MnCO3
 Rutherfordine -8.46 -22.94 -14.48 UO2CO3
 Schoepite -8.69 -2.36 6.33 UO2(OH)2:H2O
 Semetal(am) 0.11 -7.07 -7.18 Se
 Semetal(hex) 0.74 -7.07 -7.82 Se
 SeO2 -16.73 -16.61 0.12 SeO2
 SeO3 -58.66 -36.62 22.04 SeO3
 Siderite -0.30 -10.44 -10.13 FeCO3
 Thenardite -7.91 -7.53 0.38 Na2SO4
 Thermonatrite -11.35 -10.64 0.71 Na2CO3:H2O
 U3O8 -18.53 5.84 24.37 U3O8
 U4O9 -21.52 -21.64 -0.13 U4O9
 UO2(am) -11.50 -9.83 1.68 UO2
 UO2(NO3)2 -41.98 -29.26 12.71 UO2(NO3)2
 UO2(NO3)2:2H2O -34.29 -29.26 5.02 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -32.72 -29.27 3.45 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -31.17 -29.27 1.91 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -8.35 -2.36 6.00 UO2(OH)2
 UO2SeO4:4H2O -36.73 -38.98 -2.25 UO2SeO4:4H2O
 UO3 -10.61 -2.36 8.25 UO3
 Uraninite -5.68 -9.83 -4.14 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 17. SAG1-5

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

Elements	Molality	Moles
Alkalinity	3.184e-03	3.184e-03
Ca	1.070e-02	1.070e-02
Cl	8.253e-04	8.253e-04
Fe(2)	3.427e-05	3.427e-05
Fe(3)	1.794e-07	1.794e-07
K	7.663e-05	7.663e-05
Mg	2.692e-03	2.692e-03

Mn	5.454e-05	5.454e-05
Mo	8.418e-08	8.418e-08
N(-3)	1.087e-05	1.087e-05
N(5)	1.431e-06	1.431e-06
Na	3.021e-03	3.021e-03
O(0)	1.190e-05	1.190e-05
S(6)	1.346e-02	1.346e-02
Se	1.650e-09	1.650e-09
U	6.020e-09	6.020e-09

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

pH = 7.450
 pe = 1.400
 Activity of water = 0.999
 Ionic strength (mol/kgw) = 4.081e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.398e-03
 Total CO2 (mol/kg) = 3.398e-03
 Temperature (°C) = 13.20
 Electrical balance (eq) = -8.498e-04
 Percent error, 100*(Cat-|An|)/(|Cat+|An|) = -1.92
 Iterations = 21 (296 overall)
 Total H = 1.110173e+02
 Total O = 5.557087e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	1.2069	0.0686
N(-3)/N(5)	6.1716	0.3506
O(-2)/O(0)	13.6118	0.7734

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.355e-07	1.122e-07	-6.868	-6.950	-0.082	(0)	
H+	4.246e-08	3.548e-08	-7.372	-7.450	-0.078	0.00	
H2O	5.551e+01	9.995e-01	1.744	-0.000	0.000	18.03	
C(4)	3.398e-03						
HCO3-	2.974e-03	2.505e-03	-2.527	-2.601	-0.075	(0)	
H2CO3	2.328e-04	2.328e-04	-3.633	-3.633	0.000	(0)	
CaHCO3+	1.399e-04	1.185e-04	-3.854	-3.926	-0.072	(0)	
MgHCO3+	2.738e-05	2.278e-05	-4.563	-4.643	-0.080	(0)	
CaCO3	1.117e-05	1.117e-05	-4.952	-4.952	0.000	(0)	
CO3-2	5.324e-06	2.597e-06	-5.274	-5.586	-0.312	(0)	
NaHCO3	4.356e-06	4.356e-06	-5.361	-5.361	0.000	(0)	
MgCO3	1.680e-06	1.680e-06	-5.775	-5.775	0.000	(0)	
MnHCO3+	9.218e-07	7.738e-07	-6.035	-6.111	-0.076	(0)	
FeHCO3+	2.820e-07	2.387e-07	-6.550	-6.622	-0.072	(0)	
NaCO3-	1.982e-07	1.669e-07	-6.703	-6.777	-0.075	(0)	
Ca2UO2(CO3)3	5.089e-09	5.137e-09	-8.293	-8.289	0.004	(0)	
CaUO2(CO3)3-2	8.982e-10	4.381e-10	-9.047	-9.358	-0.312	(0)	
UO2(CO3)3-4	2.619e-11	6.327e-13	-10.582	-12.199	-1.617	(0)	
UO2(CO3)2-2	4.862e-12	1.917e-12	-11.313	-11.717	-0.404	(0)	
MgUO2(CO3)3-2	1.666e-12	8.128e-13	-11.778	-12.090	-0.312	(0)	
UO2CO3	4.516e-14	4.516e-14	-13.345	-13.345	0.000	(0)	
(UO2)2CO3(OH)3-	2.464e-19	2.059e-19	-18.608	-18.686	-0.078	(0)	
(UO2)3(CO3)6-6	7.026e-29	1.097e-31	-28.153	-30.960	-2.806	(0)	
Ca	1.070e-02						
Ca+2	7.260e-03	3.541e-03	-2.139	-2.451	-0.312	(0)	
CaSO4	3.290e-03	3.290e-03	-2.483	-2.483	0.000	(0)	
CaHCO3+	1.399e-04	1.185e-04	-3.854	-3.926	-0.072	(0)	

CaCO3	1.117e-05	1.117e-05	-4.952	-4.952	0.000	(0)
CaNO3+	1.825e-08	1.446e-08	-7.739	-7.840	-0.101	(0)
CaOH+	8.156e-09	6.904e-09	-8.089	-8.161	-0.072	(0)
Ca2UO2(CO3)3	5.089e-09	5.137e-09	-8.293	-8.289	0.004	(0)
CaNH3+2	1.536e-09	6.056e-10	-8.814	-9.218	-0.404	(0)
CaUO2(CO3)3-2	8.982e-10	4.381e-10	-9.047	-9.358	-0.312	(0)
Ca(NH3)2+2	8.308e-17	3.275e-17	-16.080	-16.485	-0.404	(0)
Cl	8.253e-04					
Cl-	8.253e-04	6.897e-04	-3.083	-3.161	-0.078	(0)
MnCl+	1.711e-08	1.437e-08	-7.767	-7.843	-0.076	(0)
MnCl2	1.400e-11	1.400e-11	-10.854	-10.854	0.000	(0)
MnCl3-	3.167e-15	2.659e-15	-14.499	-14.575	-0.076	(0)
FeCl+2	2.031e-19	1.009e-19	-18.692	-18.996	-0.304	(0)
UO2Cl+	5.052e-21	4.003e-21	-20.297	-20.398	-0.101	(0)
FeCl2+	5.425e-22	4.554e-22	-21.266	-21.342	-0.076	(0)
UO2Cl2	1.649e-25	1.664e-25	-24.783	-24.779	0.004	(0)
FeCl3	3.141e-26	3.141e-26	-25.503	-25.503	0.000	(0)
UCl+3	0.000e+00	0.000e+00	-40.081	-40.991	-0.910	(0)
Fe(2)	3.427e-05					
Fe+2	2.448e-05	9.649e-06	-4.611	-5.016	-0.404	(0)
FeSO4	9.462e-06	9.462e-06	-5.024	-5.024	0.000	(0)
FeHCO3+	2.820e-07	2.387e-07	-6.550	-6.622	-0.072	(0)
FeOH+	5.133e-08	4.309e-08	-7.290	-7.366	-0.076	(0)
Fe(OH)2	3.361e-12	3.361e-12	-11.474	-11.474	0.000	(0)
Fe(OH)3-	3.207e-13	2.692e-13	-12.494	-12.570	-0.076	(0)
Fe(3)	1.794e-07					
Fe(OH)2+	1.703e-07	1.434e-07	-6.769	-6.843	-0.075	(0)
Fe(OH)3	7.782e-09	7.782e-09	-8.109	-8.109	0.000	(0)
Fe(OH)4-	1.370e-09	1.154e-09	-8.863	-8.938	-0.075	(0)
FeOH+2	1.306e-12	6.487e-13	-11.884	-12.188	-0.304	(0)
FeSO4+	2.857e-16	2.398e-16	-15.544	-15.620	-0.076	(0)
Fe+3	3.570e-17	7.097e-18	-16.447	-17.149	-0.702	(0)
Fe(SO4)2-	3.251e-17	2.576e-17	-16.488	-16.589	-0.101	(0)
FeCl+2	2.031e-19	1.009e-19	-18.692	-18.996	-0.304	(0)
Fe2(OH)2+4	8.887e-22	2.147e-23	-21.051	-22.668	-1.617	(0)
FeCl2+	5.425e-22	4.554e-22	-21.266	-21.342	-0.076	(0)
FeNO3+2	3.931e-22	1.550e-22	-21.406	-21.810	-0.404	(0)
FeHSeO3+2	3.399e-23	1.340e-23	-22.469	-22.873	-0.404	(0)
FeCl3	3.141e-26	3.141e-26	-25.503	-25.503	0.000	(0)
Fe3(OH)4+5	1.318e-26	3.921e-29	-25.880	-28.407	-2.527	(0)
H(0)	3.163e-21					
H2	1.581e-21	1.596e-21	-20.801	-20.797	0.004	(0)
K	7.663e-05					
K+	7.440e-05	6.218e-05	-4.128	-4.206	-0.078	(0)
KSO4-	2.228e-06	1.876e-06	-5.652	-5.727	-0.075	(0)
Mg	2.692e-03					
Mg+2	1.947e-03	9.496e-04	-2.711	-3.022	-0.312	(0)
MgSO4	7.161e-04	7.161e-04	-3.145	-3.145	0.000	(0)
MgHCO3+	2.738e-05	2.278e-05	-4.563	-4.643	-0.080	(0)
MgCO3	1.680e-06	1.680e-06	-5.775	-5.775	0.000	(0)
MgOH+	4.088e-08	3.474e-08	-7.388	-7.459	-0.071	(0)
MgUO2(CO3)3-2	1.666e-12	8.128e-13	-11.778	-12.090	-0.312	(0)
Mn(2)	5.454e-05					
Mn+2	4.197e-05	1.655e-05	-4.377	-4.781	-0.404	(0)
MnSO4	1.162e-05	1.162e-05	-4.935	-4.935	0.000	(0)
MnHCO3+	9.218e-07	7.738e-07	-6.035	-6.111	-0.076	(0)
MnCl+	1.711e-08	1.437e-08	-7.767	-7.843	-0.076	(0)
MnOH+	5.554e-09	4.662e-09	-8.255	-8.331	-0.076	(0)
MnNO3+	3.907e-11	3.096e-11	-10.408	-10.509	-0.101	(0)
MnCl2	1.400e-11	1.400e-11	-10.854	-10.854	0.000	(0)
MnCl3-	3.167e-15	2.659e-15	-14.499	-14.575	-0.076	(0)
Mn(NO3)2	9.436e-17	9.436e-17	-16.025	-16.025	0.000	(0)
Mn(OH)3-	6.983e-18	5.862e-18	-17.156	-17.232	-0.076	(0)
MnSe	1.199e-20	1.199e-20	-19.921	-19.921	0.000	(0)
Mn(OH)4-2	1.081e-23	5.368e-24	-22.966	-23.270	-0.304	(0)
MnSeO4	9.363e-25	9.363e-25	-24.029	-24.029	0.000	(0)

Mn(3) 1.556e-29
Mn+3 1.556e-29 3.094e-30 -28.808 -29.510 -0.702 (0)
Mn(6) 0.000e+00
MnO4-2 0.000e+00 0.000e+00 -62.834 -63.138 -0.304 (0)
Mn(7) 0.000e+00
MnO4- 0.000e+00 0.000e+00 -71.831 -71.915 -0.084 (0)
Mo 8.418e-08
MoO4-2 8.416e-08 4.105e-08 -7.075 -7.387 -0.312 (0)
HMoO4- 2.623e-11 2.078e-11 -10.581 -10.682 -0.101 (0)
H2MoO4 1.160e-14 1.160e-14 -13.935 -13.935 0.000 (0)
Mo7O24-6 0.000e+00 0.000e+00 -53.032 -56.670 -3.638 (0)
HMo7O24-5 0.000e+00 0.000e+00 -55.279 -57.806 -2.527 (0)
H2Mo7O24-4 0.000e+00 0.000e+00 -58.878 -60.495 -1.617 (0)
H3Mo7O24-3 0.000e+00 0.000e+00 -63.775 -64.685 -0.910 (0)
N(-3) 1.087e-05
NH4+ 1.032e-05 8.454e-06 -4.986 -5.073 -0.087 (0)
NH4SO4- 4.924e-07 4.134e-07 -6.308 -6.384 -0.076 (0)
NH3 5.723e-08 5.723e-08 -7.242 -7.242 0.000 (0)
CaNH3+2 1.536e-09 6.056e-10 -8.814 -9.218 -0.404 (0)
Ca(NH3)2+2 8.308e-17 3.275e-17 -16.080 -16.485 -0.404 (0)
N(5) 1.431e-06
NO3- 1.413e-06 1.180e-06 -5.850 -5.928 -0.078 (0)
CaNO3+ 1.825e-08 1.446e-08 -7.739 -7.840 -0.101 (0)
MnNO3+ 3.907e-11 3.096e-11 -10.408 -10.509 -0.101 (0)
Mn(NO3)2 9.436e-17 9.436e-17 -16.025 -16.025 0.000 (0)
FeNO3+2 3.931e-22 1.550e-22 -21.406 -21.810 -0.404 (0)
UO2NO3+ 1.694e-23 1.342e-23 -22.771 -22.872 -0.101 (0)
Na 3.021e-03
Na+ 2.946e-03 2.462e-03 -2.531 -2.609 -0.078 (0)
NaSO4- 7.043e-05 5.933e-05 -4.152 -4.227 -0.075 (0)
NaHCO3 4.356e-06 4.356e-06 -5.361 -5.361 0.000 (0)
NaCO3- 1.982e-07 1.669e-07 -6.703 -6.777 -0.075 (0)
O(0) 1.190e-05
O2 5.950e-06 6.006e-06 -5.226 -5.221 0.004 (0)
S(6) 1.346e-02
SO4-2 9.356e-03 4.563e-03 -2.029 -2.341 -0.312 (0)
CaSO4 3.290e-03 3.290e-03 -2.483 -2.483 0.000 (0)
MgSO4 7.161e-04 7.161e-04 -3.145 -3.145 0.000 (0)
NaSO4- 7.043e-05 5.933e-05 -4.152 -4.227 -0.075 (0)
MnSO4 1.162e-05 1.162e-05 -4.935 -4.935 0.000 (0)
FeSO4 9.462e-06 9.462e-06 -5.024 -5.024 0.000 (0)
KSO4- 2.228e-06 1.876e-06 -5.652 -5.727 -0.075 (0)
NH4SO4- 4.924e-07 4.134e-07 -6.308 -6.384 -0.076 (0)
HSO4- 1.313e-08 1.098e-08 -7.882 -7.960 -0.078 (0)
FeSO4+ 2.857e-16 2.398e-16 -15.544 -15.620 -0.076 (0)
Fe(SO4)2- 3.251e-17 2.576e-17 -16.488 -16.589 -0.101 (0)
UO2SO4 2.313e-17 2.313e-17 -16.636 -16.636 0.000 (0)
UO2(SO4)2-2 2.616e-18 1.031e-18 -17.582 -17.987 -0.404 (0)
U(SO4)2 8.059e-35 8.059e-35 -34.094 -34.094 0.000 (0)
USO4+2 8.545e-36 3.369e-36 -35.068 -35.473 -0.404 (0)
Se(-2) 7.888e-18
HSe- 7.874e-18 6.239e-18 -17.104 -17.205 -0.101 (0)
MnSe 1.199e-20 1.199e-20 -19.921 -19.921 0.000 (0)
H2Se 1.627e-21 1.627e-21 -20.789 -20.789 0.000 (0)
Se-2 2.005e-25 7.903e-26 -24.698 -25.102 -0.404 (0)
Se(4) 1.650e-09
HSeO3- 1.366e-09 1.083e-09 -8.864 -8.966 -0.101 (0)
SeO3-2 2.835e-10 1.117e-10 -9.548 -9.952 -0.404 (0)
H2SeO3 1.478e-14 1.478e-14 -13.830 -13.830 0.000 (0)
FeHSeO3+2 3.399e-23 1.340e-23 -22.469 -22.873 -0.404 (0)
Se(6) 5.449e-22
SeO4-2 5.440e-22 2.653e-22 -21.264 -21.576 -0.312 (0)
MnSeO4 9.363e-25 9.363e-25 -24.029 -24.029 0.000 (0)
HSeO4- 4.062e-28 3.219e-28 -27.391 -27.492 -0.101 (0)
U(3) 0.000e+00
U+3 0.000e+00 0.000e+00 -49.698 -50.607 -0.910 (0)

U(4) 5.292e-17
 U(OH)5- 5.285e-17 4.187e-17 -16.277 -16.378 -0.101 (0)
 U(OH)4 7.572e-20 7.572e-20 -19.121 -19.121 0.000 (0)
 U(OH)3+ 1.437e-23 1.138e-23 -22.843 -22.944 -0.101 (0)
 U(OH)2+2 6.672e-28 2.630e-28 -27.176 -27.580 -0.404 (0)
 UOH+3 5.536e-33 6.817e-34 -32.257 -33.166 -0.910 (0)
 U(SO4)2 8.059e-35 8.059e-35 -34.094 -34.094 0.000 (0)
 USO4+2 8.545e-36 3.369e-36 -35.068 -35.473 -0.404 (0)
 U+4 8.769e-39 2.118e-40 -38.057 -39.674 -1.617 (0)
 UCl+3 0.000e+00 0.000e+00 -40.081 -40.991 -0.910 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -135.266 -143.453 -8.186 (0)
 U(5) 1.799e-16
 UO2+ 1.799e-16 1.425e-16 -15.745 -15.846 -0.101 (0)
 U(6) 6.020e-09
 Ca2UO2(CO3)3 5.089e-09 5.137e-09 -8.293 -8.289 0.004 (0)
 CaUO2(CO3)3-2 8.982e-10 4.381e-10 -9.047 -9.358 -0.312 (0)
 UO2(CO3)3-4 2.619e-11 6.327e-13 -10.582 -12.199 -1.617 (0)
 UO2(CO3)2-2 4.862e-12 1.917e-12 -11.313 -11.717 -0.404 (0)
 MgUO2(CO3)3-2 1.666e-12 8.128e-13 -11.778 -12.090 -0.312 (0)
 UO2(OH)2 1.779e-13 1.796e-13 -12.750 -12.746 0.004 (0)
 UO2CO3 4.516e-14 4.516e-14 -13.345 -13.345 0.000 (0)
 UO2(OH)3- 7.494e-15 6.263e-15 -14.125 -14.203 -0.078 (0)
 UO2OH+ 9.505e-17 7.531e-17 -16.022 -16.123 -0.101 (0)
 UO2SO4 2.313e-17 2.313e-17 -16.636 -16.636 0.000 (0)
 UO2+2 9.573e-18 4.669e-18 -17.019 -17.331 -0.312 (0)
 UO2(SO4)2-2 2.616e-18 1.031e-18 -17.582 -17.987 -0.404 (0)
 (UO2)2CO3(OH)3- 2.464e-19 2.059e-19 -18.608 -18.686 -0.078 (0)
 UO2(OH)4-2 5.637e-21 2.749e-21 -20.249 -20.561 -0.312 (0)
 UO2Cl+ 5.052e-21 4.003e-21 -20.297 -20.398 -0.101 (0)
 UO2NO3+ 1.694e-23 1.342e-23 -22.771 -22.872 -0.101 (0)
 UO2Cl2 1.649e-25 1.664e-25 -24.783 -24.779 0.004 (0)
 (UO2)2(OH)2+2 5.840e-26 2.302e-26 -25.234 -25.638 -0.404 (0)
 (UO2)3(CO3)6-6 7.026e-29 1.097e-31 -28.153 -30.960 -2.806 (0)
 (UO2)2OH+3 6.062e-30 1.205e-30 -29.217 -29.919 -0.702 (0)
 (UO2)3(OH)7- 1.525e-31 1.275e-31 -30.817 -30.895 -0.078 (0)
 (UO2)3(OH)5+ 9.832e-32 7.791e-32 -31.007 -31.108 -0.101 (0)
 (UO2)3(OH)4+2 1.548e-34 7.548e-35 -33.810 -34.122 -0.312 (0)
 (UO2)4(OH)7+ 8.965e-40 7.492e-40 -39.047 -39.125 -0.078 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-32.17	-31.72	0.45 (NH4)2SeO4
Anhydrite	-0.48	-4.79	-4.31 CaSO4
Aragonite	0.18	-8.04	-8.21 CaCO3
Artinite	-7.20	3.27	10.47 MgCO3:Mg(OH)2:3H2O
Birnessite	-16.40	1.69	18.09 MnO2
Bixbyite	-14.57	-14.32	0.25 Mn2O3
Brucite	-5.79	11.88	17.67 Mg(OH)2
Calcite	0.39	-8.04	-8.42 CaCO3
CaMoO4	-1.90	-9.84	-7.94 CaMoO4
CaSeO3:2H2O	-6.92	-3.97	2.95 CaSeO3:2H2O
CaSeO4:2H2O	-21.07	-24.03	-2.96 CaSeO4:2H2O
CH4(g)	-48.38	-91.28	-42.90 CH4
CO2(g)	-2.31	-20.49	-18.18 CO2
Dolomite(disordered)	-0.44	-16.64	-16.21 CaMg(CO3)2
Dolomite(ordered)	0.16	-16.64	-16.80 CaMg(CO3)2
Epsomite	-3.15	-5.36	-2.21 MgSO4:7H2O
Fe(OH)2	-3.68	9.88	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	5.06	2.02	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-7.57	-6.01	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-18.22	-38.84	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-39.33	-41.32	-1.99 Fe2(SO4)3
Fe3(OH)8	0.06	20.28	20.22 Fe3(OH)8
FeMoO4	-2.39	-12.40	-10.01 FeMoO4

Ferrihydrite	1.48	5.20	3.72	Fe(OH) ₃
Ferroselite	-2.79	-21.73	-18.94	FeSe ₂
FeSe	-3.76	-14.77	-11.02	FeSe
Goethite	4.27	5.20	0.93	FeOOH
Gummite	-10.69	-2.43	8.26	UO ₃
Gypsum	-0.17	-4.79	-4.62	CaSO ₄ :2H ₂ O
H-Jarosite	-8.45	-18.88	-10.43	(H ₃ O)Fe ₃ (SO ₄) ₂ (OH) ₆
H ₂ MoO ₄	-9.06	-22.29	-13.23	H ₂ MoO ₄
H ₂ Se(g)	-19.81	-24.65	-4.85	H ₂ Se
Halite	-7.35	-5.77	1.58	NaCl
Hausmannite	-16.01	48.06	64.07	Mn ₃ O ₄
Hematite	10.89	10.40	-0.49	Fe ₂ O ₃
Huntite	-4.67	-33.86	-29.19	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-15.37	-22.56	-7.19	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
K-Jarosite	-1.78	-15.64	-13.86	KFe ₃ (SO ₄) ₂ (OH) ₆
K ₂ MoO ₄	-19.09	-15.80	3.29	K ₂ MoO ₄
K ₂ SeO ₄	-29.26	-29.99	-0.73	K ₂ SeO ₄
Lepidocrocite	3.83	5.20	1.37	FeOOH
Lime	-21.65	12.45	34.10	CaO
Maghemite	4.02	10.40	6.39	Fe ₂ O ₃
Magnesioferrite	3.41	22.28	18.87	Fe ₂ MgO ₄
Magnesite	-1.00	-8.61	-7.60	MgCO ₃
Magnetite	15.38	20.29	4.91	Fe ₃ O ₄
Manganite	-6.37	18.97	25.34	MnOOH
Melanterite	-5.00	-7.36	-2.36	FeSO ₄ :7H ₂ O
Mg(OH) ₂ (active)	-6.92	11.88	18.79	Mg(OH) ₂
MgMoO ₄	-8.56	-10.41	-1.85	MgMoO ₄
MgSeO ₃ :6H ₂ O	-7.56	-4.54	3.02	MgSeO ₃ :6H ₂ O
MgSeO ₄ :6H ₂ O	-23.40	-24.60	-1.20	MgSeO ₄ :6H ₂ O
Mirabilite	-5.87	-7.56	-1.69	Na ₂ SO ₄ :10H ₂ O
Mn ₂ (SO ₄) ₃	-61.51	-66.04	-4.53	Mn ₂ (SO ₄) ₃
MnCl ₂ :4H ₂ O	-13.90	-11.10	2.79	MnCl ₂ :4H ₂ O
MnSe	-18.74	-14.54	4.21	MnSe
MnSeO ₃	-7.43	-6.30	1.13	MnSeO ₃
MnSeO ₃ :2H ₂ O	-7.22	-6.30	0.92	MnSeO ₃ :2H ₂ O
MnSeO ₄ :5H ₂ O	-24.31	-26.36	-2.05	MnSeO ₄ :5H ₂ O
MnSO ₄	-10.17	-7.12	3.05	MnSO ₄
MoO ₃	-14.29	-22.29	-8.00	MoO ₃
Na-Jarosite	-3.93	-14.04	-10.11	NaFe ₃ (SO ₄) ₂ (OH) ₆
Na ₂ Mo ₂ O ₇	-17.89	-34.89	-17.00	Na ₂ Mo ₂ O ₇
Na ₂ MoO ₄	-14.17	-12.60	1.56	Na ₂ MoO ₄
Na ₂ MoO ₄ :2H ₂ O	-13.83	-12.60	1.22	Na ₂ MoO ₄ :2H ₂ O
Na ₂ SeO ₃ :5H ₂ O	-17.03	-6.73	10.30	Na ₂ SeO ₃ :5H ₂ O
Na ₂ SeO ₄	-28.07	-26.79	1.28	Na ₂ SeO ₄
Natron	-9.02	-10.81	-1.79	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-4.11	-8.61	-4.50	MgCO ₃ :3H ₂ O
Nsutite	-15.81	1.69	17.50	MnO ₂
O ₂ (g)	-51.82	35.40	87.22	O ₂
Periclase	-10.80	11.88	22.68	MgO
Portlandite	-11.28	12.45	23.73	Ca(OH) ₂
Pyrochroite	-5.78	10.12	15.89	Mn(OH) ₂
Pyrolusite	-15.53	27.82	43.34	MnO ₂
Rhodochrosite	0.20	-10.37	-10.57	MnCO ₃
Rutherfordine	-8.44	-22.92	-14.48	UO ₂ CO ₃
Schoepite	-8.78	-2.43	6.35	UO ₂ (OH) ₂ :H ₂ O
Semetal(am)	0.23	-6.95	-7.19	Se
Semetal(hex)	0.87	-6.95	-7.82	Se
SeO ₂	-16.53	-16.42	0.11	SeO ₂
SeO ₃	-58.58	-36.48	22.10	SeO ₃
Siderite	-0.48	-10.60	-10.12	FeCO ₃
Thenardite	-7.95	-7.56	0.39	Na ₂ SO ₄
Thermonatrite	-11.52	-10.80	0.71	Na ₂ CO ₃ :H ₂ O
U ₃ O ₈	-18.81	5.78	24.59	U ₃ O ₈
U ₄ O ₉	-21.86	-21.80	0.06	U ₄ O ₉
UO ₂ (am)	-11.60	-9.87	1.73	UO ₂
UO ₂ (NO ₃) ₂	-41.94	-29.19	12.75	UO ₂ (NO ₃) ₂

UO2(NO3)2:2H2O -34.22 -29.19 5.03 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -32.64 -29.19 3.46 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -31.08 -29.19 1.90 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -8.45 -2.43 6.02 UO2(OH)2
 UO2SeO4:4H2O -36.66 -38.91 -2.25 UO2SeO4:4H2O
 UO3 -10.72 -2.43 8.28 UO3
 Uraninite -5.77 -9.87 -4.11 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 18. SAG2-1

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

Elements	Molality	Moles
Alkalinity	5.901e-03	5.901e-03
Ca	4.471e-03	4.471e-03
Cl	1.511e-03	1.511e-03
Fe(2)	7.170e-07	7.170e-07
Fe(3)	3.585e-07	3.585e-07
K	1.068e-04	1.068e-04
Mg	1.944e-03	1.944e-03
Mn	4.920e-07	4.920e-07
Mo	2.087e-08	2.087e-08
N(-3)	3.573e-06	3.573e-06
N(5)	1.708e-04	1.708e-04
Na	2.891e-03	2.891e-03
O(0)	2.184e-04	2.184e-04
S(6)	4.106e-03	4.106e-03
Se	8.063e-08	8.063e-08
U	3.007e-08	3.007e-08

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

pH = 7.350
 pe = 5.400
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.183e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 6.452e-03
 Total CO2 (mol/kg) = 6.452e-03
 Temperature (°C) = 13.90
 Electrical balance (eq) = 4.066e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.15
 Iterations = 14 (310 overall)
 Total H = 1.110207e+02
 Total O = 5.554334e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	3.2192	0.1833
N(-3)/N(5)	6.5713	0.3743
O(-2)/O(0)	13.9737	0.7959

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

Species	Molality	Log Activity	Log Molality	Log mole V	Gamma	cm ³ /mol
OH-	1.092e-07	9.436e-08	-6.962	-7.025	-0.063	(0)
H+	5.143e-08	4.467e-08	-7.289	-7.350	-0.061	0.00
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03

C(4) 6.452e-03

HCO3-	5.645e-03	4.931e-03	-2.248	-2.307	-0.059	(0)
H2CO3	5.715e-04	5.715e-04	-3.243	-3.243	0.000	(0)
CaHCO3+	1.560e-04	1.367e-04	-3.807	-3.864	-0.057	(0)
MgHCO3+	5.048e-05	4.377e-05	-4.297	-4.359	-0.062	(0)
CaCO3	1.035e-05	1.035e-05	-4.985	-4.985	0.000	(0)
NaHCO3	8.522e-06	8.522e-06	-5.069	-5.069	0.000	(0)
CO3-2	7.241e-06	4.121e-06	-5.140	-5.385	-0.245	(0)
MgCO3	2.624e-06	2.624e-06	-5.581	-5.581	0.000	(0)
NaCO3-	2.993e-07	2.615e-07	-6.524	-6.583	-0.059	(0)
Ca2UO2(CO3)3	2.368e-08	2.380e-08	-7.626	-7.624	0.002	(0)
MnHCO3+	2.213e-08	1.929e-08	-7.655	-7.715	-0.060	(0)
FeHCO3+	1.673e-08	1.466e-08	-7.776	-7.834	-0.057	(0)
CaUO2(CO3)3-2	6.209e-09	3.534e-09	-8.207	-8.452	-0.245	(0)
UO2(CO3)3-4	1.303e-10	8.531e-12	-9.885	-11.069	-1.184	(0)
UO2(CO3)2-2	3.408e-11	1.724e-11	-10.467	-10.763	-0.296	(0)
MgUO2(CO3)3-2	1.950e-11	1.110e-11	-10.710	-10.955	-0.245	(0)
UO2CO3	2.528e-13	2.528e-13	-12.597	-12.597	0.000	(0)
(UO2)2CO3(OH)3-	2.294e-18	1.993e-18	-17.639	-17.701	-0.061	(0)
(UO2)3(CO3)6-6	1.109e-26	6.955e-29	-25.955	-28.158	-2.203	(0)

Ca 4.471e-03

Ca+2	3.573e-03	2.034e-03	-2.447	-2.692	-0.245	(0)
CaSO4	7.307e-04	7.307e-04	-3.136	-3.136	0.000	(0)
CaHCO3+	1.560e-04	1.367e-04	-3.807	-3.864	-0.057	(0)
CaCO3	1.035e-05	1.035e-05	-4.985	-4.985	0.000	(0)
CaNO3+	1.222e-06	1.030e-06	-5.913	-5.987	-0.074	(0)
Ca2UO2(CO3)3	2.368e-08	2.380e-08	-7.626	-7.624	0.002	(0)
CaUO2(CO3)3-2	6.209e-09	3.534e-09	-8.207	-8.452	-0.245	(0)
CaOH+	3.839e-09	3.363e-09	-8.416	-8.473	-0.057	(0)
CaNH3+2	1.937e-10	9.801e-11	-9.713	-10.009	-0.296	(0)
Ca(NH3)2+2	2.953e-18	1.494e-18	-17.530	-17.826	-0.296	(0)

Cl 1.511e-03

Cl-	1.511e-03	1.312e-03	-2.821	-2.882	-0.061	(0)
MnCl+	3.955e-10	3.447e-10	-9.403	-9.463	-0.060	(0)
MnCl2	6.389e-13	6.389e-13	-12.195	-12.195	0.000	(0)
MnCl3-	2.649e-16	2.309e-16	-15.577	-15.637	-0.060	(0)
FeCl+2	1.124e-18	6.491e-19	-17.949	-18.188	-0.238	(0)
UO2Cl+	3.225e-20	2.720e-20	-19.492	-19.566	-0.074	(0)
FeCl2+	6.247e-21	5.446e-21	-20.204	-20.264	-0.060	(0)
UO2Cl2	2.106e-24	2.116e-24	-23.677	-23.674	0.002	(0)
FeCl3	7.146e-25	7.146e-25	-24.146	-24.146	0.000	(0)
UCl+3	0.000e+00	0.000e+00	-47.173	-47.839	-0.666	(0)

Fe(2) 7.170e-07

Fe+2	5.864e-07	2.966e-07	-6.232	-6.528	-0.296	(0)
FeSO4	1.126e-07	1.126e-07	-6.948	-6.948	0.000	(0)
FeHCO3+	1.673e-08	1.466e-08	-7.776	-7.834	-0.057	(0)
FeOH+	1.278e-09	1.114e-09	-8.893	-8.953	-0.060	(0)
Fe(OH)2	7.371e-14	7.371e-14	-13.132	-13.132	0.000	(0)
Fe(OH)3-	5.418e-15	4.724e-15	-14.266	-14.326	-0.060	(0)

Fe(3) 3.585e-07

Fe(OH)2+	3.424e-07	2.991e-07	-6.465	-6.524	-0.059	(0)
Fe(OH)3	1.434e-08	1.434e-08	-7.843	-7.843	0.000	(0)
Fe(OH)4-	1.739e-09	1.519e-09	-8.760	-8.818	-0.059	(0)
FeOH+2	3.077e-12	1.777e-12	-11.512	-11.750	-0.238	(0)
FeSO4+	3.581e-16	3.122e-16	-15.446	-15.506	-0.060	(0)
Fe+3	8.334e-17	2.345e-17	-16.079	-16.630	-0.551	(0)
Fe(SO4)2-	1.518e-17	1.280e-17	-16.819	-16.893	-0.074	(0)
FeCl+2	1.124e-18	6.491e-19	-17.949	-18.188	-0.238	(0)
FeNO3+2	1.216e-19	6.152e-20	-18.915	-19.211	-0.296	(0)
FeCl2+	6.247e-21	5.446e-21	-20.204	-20.264	-0.060	(0)
FeHSeO3+2	4.959e-21	2.508e-21	-20.305	-20.601	-0.296	(0)
Fe2(OH)2+4	2.396e-21	1.569e-22	-20.620	-21.804	-1.184	(0)
FeCl3	7.146e-25	7.146e-25	-24.146	-24.146	0.000	(0)
Fe3(OH)4+5	4.263e-26	6.025e-28	-25.370	-27.220	-1.850	(0)

H(0) 4.997e-29

H2	2.498e-29	2.511e-29	-28.602	-28.600	0.002	(0)
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K 1.068e-04
 K+ 1.055e-04 9.167e-05 -3.977 -4.038 -0.061 (0)
 KSO4- 1.221e-06 1.067e-06 -5.913 -5.972 -0.059 (0)
 Mg 1.944e-03
 Mg+2 1.622e-03 9.232e-04 -2.790 -3.035 -0.245 (0)
 MgSO4 2.689e-04 2.689e-04 -3.570 -3.570 0.000 (0)
 MgHCO3+ 5.048e-05 4.377e-05 -4.297 -4.359 -0.062 (0)
 MgCO3 2.624e-06 2.624e-06 -5.581 -5.581 0.000 (0)
 MgOH+ 3.274e-08 2.876e-08 -7.485 -7.541 -0.056 (0)
 MgUO2(CO3)3-2 1.950e-11 1.110e-11 -10.710 -10.955 -0.245 (0)
 Mn(2) 4.920e-07
 Mn+2 4.126e-07 2.087e-07 -6.385 -6.680 -0.296 (0)
 MnSO4 5.677e-08 5.677e-08 -7.246 -7.246 0.000 (0)
 MnHCO3+ 2.213e-08 1.929e-08 -7.655 -7.715 -0.060 (0)
 MnCl+ 3.955e-10 3.447e-10 -9.403 -9.463 -0.060 (0)
 MnNO3+ 5.777e-11 4.872e-11 -10.238 -10.312 -0.074 (0)
 MnOH+ 5.674e-11 4.946e-11 -10.246 -10.306 -0.060 (0)
 MnCl2 6.389e-13 6.389e-13 -12.195 -12.195 0.000 (0)
 Mn(NO3)2 1.850e-14 1.850e-14 -13.733 -13.733 0.000 (0)
 MnCl3- 2.649e-16 2.309e-16 -15.577 -15.637 -0.060 (0)
 MnSeO4 4.075e-17 4.075e-17 -16.390 -16.390 0.000 (0)
 Mn(OH)3- 4.253e-20 3.707e-20 -19.371 -19.431 -0.060 (0)
 Mn(OH)4-2 4.670e-26 2.697e-26 -25.331 -25.569 -0.238 (0)
 MnSe 0.000e+00 0.000e+00 -43.578 -43.578 0.000 (0)
 Mn(3) 1.549e-27
 Mn+3 1.549e-27 4.358e-28 -26.810 -27.361 -0.551 (0)
 Mn(6) 0.000e+00
 MnO4-2 0.000e+00 0.000e+00 -49.282 -49.520 -0.238 (0)
 Mn(7) 0.000e+00
 MnO4- 0.000e+00 0.000e+00 -54.184 -54.248 -0.065 (0)
 Mo 2.087e-08
 MoO4-2 2.086e-08 1.187e-08 -7.681 -7.925 -0.245 (0)
 HMoO4- 9.159e-12 7.724e-12 -11.038 -11.112 -0.074 (0)
 H2MoO4 5.179e-15 5.179e-15 -14.286 -14.286 0.000 (0)
 Mo7O24-6 0.000e+00 0.000e+00 -57.079 -59.743 -2.664 (0)
 HMo7O24-5 0.000e+00 0.000e+00 -58.924 -60.774 -1.850 (0)
 H2Mo7O24-4 0.000e+00 0.000e+00 -62.178 -63.362 -1.184 (0)
 H3Mo7O24-3 0.000e+00 0.000e+00 -66.787 -67.453 -0.666 (0)
 N(-3) 3.573e-06
 NH4+ 3.492e-06 2.999e-06 -5.457 -5.523 -0.066 (0)
 NH4SO4- 6.459e-08 5.631e-08 -7.190 -7.249 -0.060 (0)
 NH3 1.701e-08 1.701e-08 -7.769 -7.769 0.000 (0)
 CaNH3+2 1.937e-10 9.801e-11 -9.713 -10.009 -0.296 (0)
 Ca(NH3)2+2 2.953e-18 1.494e-18 -17.530 -17.826 -0.296 (0)
 N(5) 1.708e-04
 NO3- 1.696e-04 1.473e-04 -3.771 -3.832 -0.061 (0)
 CaNO3+ 1.222e-06 1.030e-06 -5.913 -5.987 -0.074 (0)
 MnNO3+ 5.777e-11 4.872e-11 -10.238 -10.312 -0.074 (0)
 Mn(NO3)2 1.850e-14 1.850e-14 -13.733 -13.733 0.000 (0)
 FeNO3+2 1.216e-19 6.152e-20 -18.915 -19.211 -0.296 (0)
 UO2NO3+ 6.893e-21 5.813e-21 -20.162 -20.236 -0.074 (0)
 Na 2.891e-03
 Na+ 2.856e-03 2.481e-03 -2.544 -2.605 -0.061 (0)
 NaSO4- 2.631e-05 2.298e-05 -4.580 -4.639 -0.059 (0)
 NaHCO3 8.522e-06 8.522e-06 -5.069 -5.069 0.000 (0)
 NaCO3- 2.993e-07 2.615e-07 -6.524 -6.583 -0.059 (0)
 O(0) 2.184e-04
 O2 1.092e-04 1.097e-04 -3.962 -3.960 0.002 (0)
 S(6) 4.106e-03
 SO4-2 3.078e-03 1.752e-03 -2.512 -2.756 -0.245 (0)
 CaSO4 7.307e-04 7.307e-04 -3.136 -3.136 0.000 (0)
 MgSO4 2.689e-04 2.689e-04 -3.570 -3.570 0.000 (0)
 NaSO4- 2.631e-05 2.298e-05 -4.580 -4.639 -0.059 (0)
 KSO4- 1.221e-06 1.067e-06 -5.913 -5.972 -0.059 (0)
 FeSO4 1.126e-07 1.126e-07 -6.948 -6.948 0.000 (0)
 NH4SO4- 6.459e-08 5.631e-08 -7.190 -7.249 -0.060 (0)

MnSO4	5.677e-08	5.677e-08	-7.246	-7.246	0.000	(0)
HSO4-	6.242e-09	5.427e-09	-8.205	-8.265	-0.061	(0)
FeSO4+	3.581e-16	3.122e-16	-15.446	-15.506	-0.060	(0)
UO2SO4	3.184e-17	3.184e-17	-16.497	-16.497	0.000	(0)
Fe(SO4)2-	1.518e-17	1.280e-17	-16.819	-16.893	-0.074	(0)
UO2(SO4)2-2	1.098e-18	5.554e-19	-17.959	-18.255	-0.296	(0)
U(SO4)2	0.000e+00	0.000e+00	-42.029	-42.029	0.000	(0)
USO4+2	0.000e+00	0.000e+00	-42.707	-43.003	-0.296	(0)
Se(-2)	1.626e-39					
HSe-	1.626e-39	1.371e-39	-38.789	-38.863	-0.074	(0)
H2Se	0.000e+00	0.000e+00	-42.345	-42.345	0.000	(0)
MnSe	0.000e+00	0.000e+00	-43.578	-43.578	0.000	(0)
Se-2	0.000e+00	0.000e+00	-46.543	-46.839	-0.296	(0)
Se(4)	8.063e-08					
HSeO3-	7.089e-08	5.978e-08	-7.149	-7.223	-0.074	(0)
SeO3-2	9.740e-09	4.927e-09	-8.011	-8.307	-0.296	(0)
H2SeO3	1.034e-12	1.034e-12	-11.985	-11.985	0.000	(0)
FeHSeO3+2	4.959e-21	2.508e-21	-20.305	-20.601	-0.296	(0)
Se(6)	1.586e-12					
SeO4-2	1.586e-12	9.025e-13	-11.800	-12.045	-0.245	(0)
MnSeO4	4.075e-17	4.075e-17	-16.390	-16.390	0.000	(0)
HSeO4-	1.673e-18	1.411e-18	-17.776	-17.850	-0.074	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-61.014	-61.680	-0.666	(0)
U(4)	1.349e-24					
U(OH)5-	1.346e-24	1.135e-24	-23.871	-23.945	-0.074	(0)
U(OH)4	2.553e-27	2.553e-27	-26.593	-26.593	0.000	(0)
U(OH)3+	5.677e-31	4.787e-31	-30.246	-30.320	-0.074	(0)
U(OH)2+2	2.695e-35	1.363e-35	-34.569	-34.865	-0.296	(0)
UOH+3	2.006e-40	0.000e+00	-39.698	-40.364	-0.666	(0)
U(SO4)2	0.000e+00	0.000e+00	-42.029	-42.029	0.000	(0)
USO4+2	0.000e+00	0.000e+00	-42.707	-43.003	-0.296	(0)
U+4	0.000e+00	0.000e+00	-45.609	-46.793	-1.184	(0)
UCl+3	0.000e+00	0.000e+00	-47.173	-47.839	-0.666	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-181.670	-187.663	-5.993	(0)
U(5)	5.853e-20					
UO2+	5.853e-20	4.936e-20	-19.233	-19.307	-0.074	(0)
U(6)	3.007e-08					
Ca2UO2(CO3)3	2.368e-08	2.380e-08	-7.626	-7.624	0.002	(0)
CaUO2(CO3)3-2	6.209e-09	3.534e-09	-8.207	-8.452	-0.245	(0)
UO2(CO3)3-4	1.303e-10	8.531e-12	-9.885	-11.069	-1.184	(0)
UO2(CO3)2-2	3.408e-11	1.724e-11	-10.467	-10.763	-0.296	(0)
MgUO2(CO3)3-2	1.950e-11	1.110e-11	-10.710	-10.955	-0.245	(0)
UO2(OH)2	3.961e-13	3.981e-13	-12.402	-12.400	0.002	(0)
UO2CO3	2.528e-13	2.528e-13	-12.597	-12.597	0.000	(0)
UO2(OH)3-	1.270e-14	1.103e-14	-13.896	-13.957	-0.061	(0)
UO2OH+	2.617e-16	2.207e-16	-15.582	-15.656	-0.074	(0)
UO2SO4	3.184e-17	3.184e-17	-16.497	-16.497	0.000	(0)
UO2+2	2.882e-17	1.640e-17	-16.540	-16.785	-0.245	(0)
(UO2)2CO3(OH)3-	2.294e-18	1.993e-18	-17.639	-17.701	-0.061	(0)
UO2(SO4)2-2	1.098e-18	5.554e-19	-17.959	-18.255	-0.296	(0)
UO2Cl+	3.225e-20	2.720e-20	-19.492	-19.566	-0.074	(0)
UO2NO3+	6.893e-21	5.813e-21	-20.162	-20.236	-0.074	(0)
UO2(OH)4-2	6.760e-21	3.848e-21	-20.170	-20.415	-0.245	(0)
UO2Cl2	2.106e-24	2.116e-24	-23.677	-23.674	0.002	(0)
(UO2)2(OH)2+2	3.700e-25	1.872e-25	-24.432	-24.728	-0.296	(0)
(UO2)3(CO3)6-6	1.109e-26	6.955e-29	-25.955	-28.158	-2.203	(0)
(UO2)2OH+3	4.199e-29	1.182e-29	-28.377	-28.928	-0.551	(0)
(UO2)3(OH)5+	1.416e-30	1.194e-30	-29.849	-29.923	-0.074	(0)
(UO2)3(OH)7-	1.271e-30	1.104e-30	-29.896	-29.957	-0.061	(0)
(UO2)3(OH)4+2	2.290e-33	1.304e-33	-32.640	-32.885	-0.245	(0)
(UO2)4(OH)7+	2.624e-38	2.279e-38	-37.581	-37.642	-0.061	(0)

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

Phase SI** log IAP log K(287 K, 1 atm)

(NH4)2SeO4 -23.54 -23.09 0.45 (NH4)2SeO4
 Anhydrite -1.14 -5.45 -4.31 CaSO4
 Aragonite 0.14 -8.08 -8.22 CaCO3
 Artinite -7.17 3.24 10.41 MgCO3:Mg(OH)2:3H2O
 Birnessite -10.65 7.44 18.09 MnO2
 Bixbyite -10.82 -10.62 0.20 Mn2O3
 Brucite -5.95 11.66 17.62 Mg(OH)2
 Calcite 0.35 -8.08 -8.43 CaCO3
 CaMoO4 -2.68 -10.62 -7.94 CaMoO4
 CaSeO3:2H2O -5.51 -2.57 2.95 CaSeO3:2H2O
 CaSeO4:2H2O -11.77 -14.74 -2.96 CaSeO4:2H2O
 CH4(g) -79.30 -122.08 -42.79 CH4
 CO2(g) -1.91 -20.08 -18.17 CO2
 Dolomite(disordered) -0.27 -16.50 -16.23 CaMg(CO3)2
 Dolomite(ordered) 0.33 -16.50 -16.82 CaMg(CO3)2
 Epsomite -3.59 -5.79 -2.20 MgSO4:7H2O
 Fe(OH)2 -5.39 8.17 13.56 Fe(OH)2
 Fe(OH)2.7Cl.3 5.39 2.35 -3.04 Fe(OH)2.7Cl.3
 Fe2(OH)4SeO3 -5.29 -3.73 1.55 Fe2(OH)4SeO3
 Fe2(SeO3)3:2H2O -12.25 -32.88 -20.63 Fe2(SeO3)3:2H2O
 Fe2(SO4)3 -39.43 -41.53 -2.09 Fe2(SO4)3
 Fe3(OH)8 -1.21 19.01 20.22 Fe3(OH)8
 FeMoO4 -4.44 -14.45 -10.02 FeMoO4
 Ferrihydrite 1.73 5.42 3.69 Fe(OH)3
 Ferroselite -39.84 -58.75 -18.92 FeSe2
 FeSe -27.03 -38.04 -11.01 FeSe
 Goethite 4.52 5.42 0.90 FeOOH
 Gummite -10.31 -2.09 8.22 UO3
 Gypsum -0.83 -5.45 -4.62 CaSO4:2H2O
 H-Jarosite -8.12 -18.65 -10.54 (H3O)Fe3(SO4)2(OH)6
 H2MoO4 -9.42 -22.63 -13.21 H2MoO4
 H2Se(g) -41.36 -46.21 -4.86 H2Se
 Halite -7.06 -5.49 1.58 NaCl
 Hausmannite -14.32 49.56 63.88 Mn3O4
 Hematite 11.38 10.84 -0.54 Fe2O3
 Huntite -4.10 -33.34 -29.24 CaMg3(CO3)4
 Hydromagnesite -14.73 -22.01 -7.29 Mg5(CO3)4(OH)2:4H2O
 K-Jarosite -1.43 -15.34 -13.91 KFe3(SO4)2(OH)6
 K2MoO4 -19.29 -16.00 3.28 K2MoO4
 K2SeO4 -19.39 -20.12 -0.73 K2SeO4
 Lepidocrocite 4.05 5.42 1.37 FeOOH
 Lime -22.00 12.01 34.01 CaO
 Maghemite 4.45 10.84 6.39 Fe2O3
 Magnesioferrite 3.76 22.51 18.75 Fe2MgO4
 Magnesite -0.82 -8.42 -7.60 MgCO3
 Magnetite 14.20 19.01 4.82 Fe3O4
 Manganite -4.57 20.77 25.34 MnOOH
 Melanterite -6.94 -9.29 -2.35 FeSO4:7H2O
 Mg(OH)2(active) -7.13 11.66 18.79 Mg(OH)2
 MgMoO4 -9.11 -10.96 -1.85 MgMoO4
 MgSeO3:6H2O -5.93 -2.91 3.02 MgSeO3:6H2O
 MgSeO4:6H2O -13.88 -15.08 -1.20 MgSeO4:6H2O
 Mirabilite -6.32 -7.97 -1.65 Na2SO4:10H2O
 Mn2(SO4)3 -58.39 -62.99 -4.60 Mn2(SO4)3
 MnCl2:4H2O -15.23 -12.45 2.79 MnCl2:4H2O
 MnSe -42.36 -38.19 4.16 MnSe
 MnSeO3 -7.68 -6.55 1.13 MnSeO3
 MnSeO3:2H2O -7.48 -6.55 0.92 MnSeO3:2H2O
 MnSeO4:5H2O -16.68 -18.73 -2.05 MnSeO4:5H2O
 MnSO4 -12.46 -9.44 3.02 MnSO4
 MoO3 -14.63 -22.63 -8.00 MoO3
 Na-Jarosite -3.73 -13.91 -10.17 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -18.78 -35.76 -16.98 Na2Mo2O7
 Na2MoO4 -14.69 -13.14 1.56 Na2MoO4
 Na2MoO4:2H2O -14.36 -13.14 1.22 Na2MoO4:2H2O

Na2SeO3:5H2O -15.38 -5.08 10.30 Na2SeO3:5H2O
 Na2SeO4 -18.54 -17.26 1.28 Na2SeO4
 Natron -8.84 -10.60 -1.76 Na2CO3:10H2O
 Nesquehonite -3.91 -8.42 -4.51 MgCO3:3H2O
 Nsutite -10.07 7.44 17.50 MnO2
 O2(g) -35.96 51.00 86.96 O2
 Periclase -10.94 11.67 22.61 MgO
 Portlandite -11.67 12.01 23.68 Ca(OH)2
 Pyrochroite -7.83 8.02 15.85 Mn(OH)2
 Pyrolusite -9.70 33.52 43.22 MnO2
 Rhodochrosite -1.50 -12.07 -10.57 MnCO3
 Rutherfordine -7.69 -22.17 -14.48 UO2CO3
 Schoepite -8.42 -2.09 6.33 UO2(OH)2:H2O
 Semetal(am) -13.53 -20.71 -7.18 Se
 Semetal(hex) -12.90 -20.71 -7.82 Se
 SeO2 -14.69 -14.57 0.12 SeO2
 SeO3 -48.78 -26.74 22.04 SeO3
 Siderite -1.78 -11.91 -10.13 FeCO3
 Thenardite -8.35 -7.97 0.38 Na2SO4
 Thermonatrite -11.30 -10.60 0.71 Na2CO3:H2O
 U3O8 -25.55 -1.18 24.37 U3O8
 U4O9 -43.94 -44.07 -0.13 U4O9
 UO2(am) -19.07 -17.39 1.68 UO2
 UO2(NO3)2 -37.16 -24.45 12.71 UO2(NO3)2
 UO2(NO3)2:2H2O -29.47 -24.45 5.02 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -27.90 -24.45 3.45 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -26.35 -24.45 1.91 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -8.08 -2.09 6.00 UO2(OH)2
 UO2SeO4:4H2O -26.58 -28.83 -2.25 UO2SeO4:4H2O
 UO3 -10.33 -2.09 8.25 UO3
 Uraninite -13.25 -17.39 -4.14 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 19. SAG2-2

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

Elements	Molality	Moles
Alkalinity	5.841e-03	5.841e-03
Ca	4.421e-03	4.421e-03
Cl	1.525e-03	1.525e-03
Fe(2)	1.255e-06	1.255e-06
Fe(3)	1.075e-06	1.075e-06
K	1.034e-04	1.034e-04
Mg	1.944e-03	1.944e-03
Mn	5.466e-07	5.466e-07
Mo	3.057e-08	3.057e-08
N(-3)	3.573e-06	3.573e-06
N(5)	1.594e-04	1.594e-04
Na	2.874e-03	2.874e-03
O(0)	1.489e-04	1.489e-04
S(6)	3.970e-03	3.970e-03
Se	7.188e-08	7.188e-08
U	3.024e-08	3.024e-08

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

pH = 7.380
 pe = 5.200
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.156e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 6.349e-03

Total CO2 (mol/kg) = 6.349e-03
 Temperature (°C) = 13.60
 Electrical balance (eq) = 2.501e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.93
 Iterations = 16 (326 overall)
 Total H = 1.110205e+02
 Total O = 5.554239e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	3.3970	0.1933
N(-3)/N(5)	6.5487	0.3726
O(-2)/O(0)	13.9250	0.7923

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.140e-07	9.866e-08	-6.943	-7.006	-0.063	(0)	
H+	4.796e-08	4.169e-08	-7.319	-7.380	-0.061	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	
C(4)	6.349e-03						
HCO3-	5.586e-03	4.883e-03	-2.253	-2.311	-0.058	(0)	
H2CO3	5.303e-04	5.303e-04	-3.275	-3.275	0.000	(0)	
CaHCO3+	1.526e-04	1.338e-04	-3.816	-3.874	-0.057	(0)	
MgHCO3+	5.024e-05	4.359e-05	-4.299	-4.361	-0.062	(0)	
CaCO3	1.081e-05	1.081e-05	-4.966	-4.966	0.000	(0)	
NaHCO3	8.448e-06	8.448e-06	-5.073	-5.073	0.000	(0)	
CO3-2	7.611e-06	4.346e-06	-5.119	-5.362	-0.243	(0)	
MgCO3	2.773e-06	2.773e-06	-5.557	-5.557	0.000	(0)	
NaCO3-	3.166e-07	2.768e-07	-6.499	-6.558	-0.058	(0)	
FeHCO3+	2.907e-08	2.549e-08	-7.537	-7.594	-0.057	(0)	
MnHCO3+	2.449e-08	2.137e-08	-7.611	-7.670	-0.059	(0)	
Ca2UO2(CO3)3	2.381e-08	2.393e-08	-7.623	-7.621	0.002	(0)	
CaUO2(CO3)3-2	6.242e-09	3.564e-09	-8.205	-8.448	-0.243	(0)	
UO2(CO3)3-4	1.317e-10	8.779e-12	-9.881	-11.057	-1.176	(0)	
UO2(CO3)2-2	3.231e-11	1.642e-11	-10.491	-10.785	-0.294	(0)	
MgUO2(CO3)3-2	1.980e-11	1.131e-11	-10.703	-10.947	-0.243	(0)	
UO2CO3	2.296e-13	2.296e-13	-12.639	-12.639	0.000	(0)	
(UO2)2CO3(OH)3-	2.227e-18	1.936e-18	-17.652	-17.713	-0.061	(0)	
(UO2)3(CO3)6-6	9.889e-27	6.375e-29	-26.005	-28.196	-2.191	(0)	
Ca	4.421e-03						
Ca+2	3.552e-03	2.028e-03	-2.450	-2.693	-0.243	(0)	
CaSO4	7.045e-04	7.045e-04	-3.152	-3.152	0.000	(0)	
CaHCO3+	1.526e-04	1.338e-04	-3.816	-3.874	-0.057	(0)	
CaCO3	1.081e-05	1.081e-05	-4.966	-4.966	0.000	(0)	
CaNO3+	1.139e-06	9.618e-07	-5.943	-6.017	-0.073	(0)	
Ca2UO2(CO3)3	2.381e-08	2.393e-08	-7.623	-7.621	0.002	(0)	
CaUO2(CO3)3-2	6.242e-09	3.564e-09	-8.205	-8.448	-0.243	(0)	
CaOH+	3.985e-09	3.494e-09	-8.400	-8.457	-0.057	(0)	
CaNH3+2	2.063e-10	1.048e-10	-9.685	-9.979	-0.294	(0)	
Ca(NH3)2+2	3.374e-18	1.714e-18	-17.472	-17.766	-0.294	(0)	
Cl	1.525e-03						
Cl-	1.525e-03	1.325e-03	-2.817	-2.878	-0.061	(0)	
MnCl+	4.472e-10	3.901e-10	-9.350	-9.409	-0.059	(0)	
MnCl2	7.303e-13	7.303e-13	-12.136	-12.136	0.000	(0)	
MnCl3-	3.056e-16	2.666e-16	-15.515	-15.574	-0.059	(0)	
FeCl+2	2.925e-18	1.694e-18	-17.534	-17.771	-0.237	(0)	
UO2Cl+	2.787e-20	2.353e-20	-19.555	-19.628	-0.073	(0)	
FeCl2+	1.663e-20	1.450e-20	-19.779	-19.838	-0.059	(0)	
FeCl3	1.922e-24	1.922e-24	-23.716	-23.716	0.000	(0)	
UO2Cl2	1.853e-24	1.863e-24	-23.732	-23.730	0.002	(0)	
UCl+3	0.000e+00	0.000e+00	-46.926	-47.588	-0.661	(0)	

Fe(2) 1.255e-06
 Fe+2 1.031e-06 5.239e-07 -5.987 -6.281 -0.294 (0)
 FeSO4 1.923e-07 1.923e-07 -6.716 -6.716 0.000 (0)
 FeHCO3+ 2.907e-08 2.549e-08 -7.537 -7.594 -0.057 (0)
 FeOH+ 2.359e-09 2.058e-09 -8.627 -8.687 -0.059 (0)
 Fe(OH)2 1.419e-13 1.419e-13 -12.848 -12.848 0.000 (0)
 Fe(OH)3- 1.113e-14 9.711e-15 -13.953 -14.013 -0.059 (0)
 Fe(3) 1.075e-06
 Fe(OH)2+ 1.025e-06 8.965e-07 -5.989 -6.047 -0.058 (0)
 Fe(OH)3 4.400e-08 4.400e-08 -7.357 -7.357 0.000 (0)
 Fe(OH)4- 5.979e-09 5.227e-09 -8.223 -8.282 -0.058 (0)
 FeOH+2 8.426e-12 4.881e-12 -11.074 -11.311 -0.237 (0)
 FeSO4+ 8.960e-16 7.817e-16 -15.048 -15.107 -0.059 (0)
 Fe+3 2.160e-16 6.121e-17 -15.665 -16.213 -0.548 (0)
 Fe(SO4)2- 3.692e-17 3.117e-17 -16.433 -16.506 -0.073 (0)
 FeCl+2 2.925e-18 1.694e-18 -17.534 -17.771 -0.237 (0)
 FeNO3+2 2.999e-19 1.524e-19 -18.523 -18.817 -0.294 (0)
 Fe2(OH)2+4 1.795e-20 1.197e-21 -19.746 -20.922 -1.176 (0)
 FeCl2+ 1.663e-20 1.450e-20 -19.779 -19.838 -0.059 (0)
 FeHSeO3+2 1.129e-20 5.735e-21 -19.947 -20.241 -0.294 (0)
 FeCl3 1.922e-24 1.922e-24 -23.716 -23.716 0.000 (0)
 Fe3(OH)4+5 9.442e-25 1.373e-26 -24.025 -25.862 -1.837 (0)
 H(0) 1.097e-28
 H2 5.484e-29 5.511e-29 -28.261 -28.259 0.002 (0)
 K 1.034e-04
 K+ 1.023e-04 8.892e-05 -3.990 -4.051 -0.061 (0)
 KSO4- 1.146e-06 1.002e-06 -5.941 -5.999 -0.058 (0)
 Mg 1.944e-03
 Mg+2 1.629e-03 9.300e-04 -2.788 -3.032 -0.243 (0)
 MgSO4 2.621e-04 2.621e-04 -3.582 -3.582 0.000 (0)
 MgHCO3+ 5.024e-05 4.359e-05 -4.299 -4.361 -0.062 (0)
 MgCO3 2.773e-06 2.773e-06 -5.557 -5.557 0.000 (0)
 MgOH+ 3.428e-08 3.013e-08 -7.465 -7.521 -0.056 (0)
 MgUO2(CO3)3-2 1.980e-11 1.131e-11 -10.703 -10.947 -0.243 (0)
 Mn(2) 5.466e-07
 Mn+2 4.601e-07 2.338e-07 -6.337 -6.631 -0.294 (0)
 MnSO4 6.146e-08 6.146e-08 -7.211 -7.211 0.000 (0)
 MnHCO3+ 2.449e-08 2.137e-08 -7.611 -7.670 -0.059 (0)
 MnCl+ 4.472e-10 3.901e-10 -9.350 -9.409 -0.059 (0)
 MnOH+ 6.642e-11 5.794e-11 -10.178 -10.237 -0.059 (0)
 MnNO3+ 6.037e-11 5.097e-11 -10.219 -10.293 -0.073 (0)
 MnCl2 7.303e-13 7.303e-13 -12.136 -12.136 0.000 (0)
 Mn(NO3)2 1.808e-14 1.808e-14 -13.743 -13.743 0.000 (0)
 MnCl3- 3.056e-16 2.666e-16 -15.515 -15.574 -0.059 (0)
 MnSeO4 1.802e-17 1.802e-17 -16.744 -16.744 0.000 (0)
 Mn(OH)3- 5.857e-20 5.110e-20 -19.232 -19.292 -0.059 (0)
 Mn(OH)4-2 6.877e-26 3.983e-26 -25.163 -25.400 -0.237 (0)
 MnSe 0.000e+00 0.000e+00 -42.532 -42.532 0.000 (0)
 Mn(3) 1.037e-27
 Mn+3 1.037e-27 2.938e-28 -26.984 -27.532 -0.548 (0)
 Mn(6) 0.000e+00
 MnO4-2 0.000e+00 0.000e+00 -49.929 -50.166 -0.237 (0)
 Mn(7) 0.000e+00
 MnO4- 0.000e+00 0.000e+00 -55.051 -55.115 -0.064 (0)
 Mo 3.057e-08
 MoO4-2 3.056e-08 1.745e-08 -7.515 -7.758 -0.243 (0)
 HMoO4- 1.244e-11 1.050e-11 -10.905 -10.979 -0.073 (0)
 H2MoO4 6.705e-15 6.705e-15 -14.174 -14.174 0.000 (0)
 Mo7O24-6 0.000e+00 0.000e+00 -56.123 -58.769 -2.646 (0)
 HMo7O24-5 0.000e+00 0.000e+00 -57.995 -59.832 -1.837 (0)
 H2Mo7O24-4 0.000e+00 0.000e+00 -61.275 -62.451 -1.176 (0)
 H3Mo7O24-3 0.000e+00 0.000e+00 -65.909 -66.571 -0.661 (0)
 N(-3) 3.573e-06
 NH4+ 3.493e-06 3.003e-06 -5.457 -5.522 -0.066 (0)
 NH4SO4- 6.268e-08 5.468e-08 -7.203 -7.262 -0.059 (0)
 NH3 1.784e-08 1.784e-08 -7.749 -7.749 0.000 (0)

CaNH3+2	2.063e-10	1.048e-10	-9.685	-9.979	-0.294	(0)
Ca(NH3)2+2	3.374e-18	1.714e-18	-17.472	-17.766	-0.294	(0)
N(5)	1.594e-04					
NO3-	1.582e-04	1.375e-04	-3.801	-3.862	-0.061	(0)
CaNO3+	1.139e-06	9.618e-07	-5.943	-6.017	-0.073	(0)
MnNO3+	6.037e-11	5.097e-11	-10.219	-10.293	-0.073	(0)
Mn(NO3)2	1.808e-14	1.808e-14	-13.743	-13.743	0.000	(0)
FeNO3+2	2.999e-19	1.524e-19	-18.523	-18.817	-0.294	(0)
UO2NO3+	5.575e-21	4.707e-21	-20.254	-20.327	-0.073	(0)
Na	2.874e-03					
Na+	2.840e-03	2.468e-03	-2.547	-2.608	-0.061	(0)
NaSO4-	2.536e-05	2.217e-05	-4.596	-4.654	-0.058	(0)
NaHCO3	8.448e-06	8.448e-06	-5.073	-5.073	0.000	(0)
NaCO3-	3.166e-07	2.768e-07	-6.499	-6.558	-0.058	(0)
O(0)	1.489e-04					
O2	7.445e-05	7.482e-05	-4.128	-4.126	0.002	(0)
S(6)	3.970e-03					
SO4-2	2.977e-03	1.699e-03	-2.526	-2.770	-0.243	(0)
CaSO4	7.045e-04	7.045e-04	-3.152	-3.152	0.000	(0)
MgSO4	2.621e-04	2.621e-04	-3.582	-3.582	0.000	(0)
NaSO4-	2.536e-05	2.217e-05	-4.596	-4.654	-0.058	(0)
KSO4-	1.146e-06	1.002e-06	-5.941	-5.999	-0.058	(0)
FeSO4	1.923e-07	1.923e-07	-6.716	-6.716	0.000	(0)
NH4SO4-	6.268e-08	5.468e-08	-7.203	-7.262	-0.059	(0)
MnSO4	6.146e-08	6.146e-08	-7.211	-7.211	0.000	(0)
HSO4-	5.592e-09	4.865e-09	-8.252	-8.313	-0.060	(0)
FeSO4+	8.960e-16	7.817e-16	-15.048	-15.107	-0.059	(0)
Fe(SO4)2-	3.692e-17	3.117e-17	-16.433	-16.506	-0.073	(0)
UO2SO4	2.641e-17	2.641e-17	-16.578	-16.578	0.000	(0)
UO2(SO4)2-2	8.724e-19	4.433e-19	-18.059	-18.353	-0.294	(0)
U(SO4)2	0.000e+00	0.000e+00	-41.819	-41.819	0.000	(0)
USO4+2	0.000e+00	0.000e+00	-42.481	-42.775	-0.294	(0)
Se(-2)	1.506e-38					
HSe-	1.506e-38	1.271e-38	-37.822	-37.896	-0.073	(0)
H2Se	0.000e+00	0.000e+00	-41.409	-41.409	0.000	(0)
MnSe	0.000e+00	0.000e+00	-42.532	-42.532	0.000	(0)
Se-2	0.000e+00	0.000e+00	-45.557	-45.851	-0.294	(0)
Se(4)	7.188e-08					
HSeO3-	6.270e-08	5.294e-08	-7.203	-7.276	-0.073	(0)
SeO3-2	9.179e-09	4.665e-09	-8.037	-8.331	-0.294	(0)
H2SeO3	8.523e-13	8.523e-13	-12.069	-12.069	0.000	(0)
FeHSeO3+2	1.129e-20	5.735e-21	-19.947	-20.241	-0.294	(0)
Se(6)	6.277e-13					
SeO4-2	6.277e-13	3.584e-13	-12.202	-12.446	-0.243	(0)
MnSeO4	1.802e-17	1.802e-17	-16.744	-16.744	0.000	(0)
HSeO4-	6.132e-19	5.178e-19	-18.212	-18.286	-0.073	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-60.595	-61.256	-0.661	(0)
U(4)	3.167e-24					
U(OH)5-	3.161e-24	2.669e-24	-23.500	-23.574	-0.073	(0)
U(OH)4	5.630e-27	5.630e-27	-26.249	-26.249	0.000	(0)
U(OH)3+	1.172e-30	9.893e-31	-29.931	-30.005	-0.073	(0)
U(OH)2+2	5.220e-35	2.653e-35	-34.282	-34.576	-0.294	(0)
UOH+3	3.648e-40	0.000e+00	-39.438	-40.099	-0.661	(0)
U(SO4)2	0.000e+00	0.000e+00	-41.819	-41.819	0.000	(0)
USO4+2	0.000e+00	0.000e+00	-42.481	-42.775	-0.294	(0)
U+4	0.000e+00	0.000e+00	-45.373	-46.549	-1.176	(0)
UCl+3	0.000e+00	0.000e+00	-46.926	-47.588	-0.661	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-179.800	-185.753	-5.953	(0)
U(5)	8.042e-20					
UO2+	8.042e-20	6.790e-20	-19.095	-19.168	-0.073	(0)
U(6)	3.024e-08					
Ca2UO2(CO3)3	2.381e-08	2.393e-08	-7.623	-7.621	0.002	(0)
CaUO2(CO3)3-2	6.242e-09	3.564e-09	-8.205	-8.448	-0.243	(0)
UO2(CO3)3-4	1.317e-10	8.779e-12	-9.881	-11.057	-1.176	(0)
UO2(CO3)2-2	3.231e-11	1.642e-11	-10.491	-10.785	-0.294	(0)

MgUO2(CO3)3-2 1.980e-11 1.131e-11 -10.703 -10.947 -0.243 (0)
UO2(OH)2 3.924e-13 3.943e-13 -12.406 -12.404 0.002 (0)
UO2CO3 2.296e-13 2.296e-13 -12.639 -12.639 0.000 (0)
UO2(OH)3- 1.347e-14 1.171e-14 -13.871 -13.932 -0.061 (0)
UO2OH+ 2.366e-16 1.998e-16 -15.626 -15.699 -0.073 (0)
UO2SO4 2.641e-17 2.641e-17 -16.578 -16.578 0.000 (0)
UO2+2 2.478e-17 1.415e-17 -16.606 -16.849 -0.243 (0)
(UO2)2CO3(OH)3- 2.227e-18 1.936e-18 -17.652 -17.713 -0.061 (0)
UO2(SO4)2-2 8.724e-19 4.433e-19 -18.059 -18.353 -0.294 (0)
UO2Cl+ 2.787e-20 2.353e-20 -19.555 -19.628 -0.073 (0)
UO2(OH)4-2 7.664e-21 4.376e-21 -20.116 -20.359 -0.243 (0)
UO2NO3+ 5.575e-21 4.707e-21 -20.254 -20.327 -0.073 (0)
UO2Cl2 1.853e-24 1.863e-24 -23.732 -23.730 0.002 (0)
(UO2)2(OH)2+2 3.090e-25 1.570e-25 -24.510 -24.804 -0.294 (0)
(UO2)3(CO3)6-6 9.889e-27 6.375e-29 -26.005 -28.196 -2.191 (0)
(UO2)2OH+3 3.325e-29 9.421e-30 -28.478 -29.026 -0.548 (0)
(UO2)3(OH)7- 1.322e-30 1.149e-30 -29.879 -29.940 -0.061 (0)
(UO2)3(OH)5+ 1.223e-30 1.033e-30 -29.913 -29.986 -0.073 (0)
(UO2)3(OH)4+2 1.932e-33 1.103e-33 -32.714 -32.957 -0.243 (0)
(UO2)4(OH)7+ 2.355e-38 2.047e-38 -37.628 -37.689 -0.061 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-23.94	-23.49	0.45 (NH4)2SeO4
Anhydrite	-1.15	-5.46	-4.31 CaSO4
Aragonite	0.16	-8.05	-8.22 CaCO3
Artinite	-7.10	3.33	10.44 MgCO3:Mg(OH)2:3H2O
Birnessite	-10.90	7.19	18.09 MnO2
Bixbyite	-11.01	-10.78	0.22 Mn2O3
Brucite	-5.91	11.73	17.64 Mg(OH)2
Calcite	0.37	-8.05	-8.42 CaCO3
CaMoO4	-2.52	-10.45	-7.94 CaMoO4
CaSeO3:2H2O	-5.54	-2.59	2.95 CaSeO3:2H2O
CaSeO4:2H2O	-12.18	-15.14	-2.96 CaSeO4:2H2O
CH4(g)	-77.93	-120.76	-42.84 CH4
CO2(g)	-1.95	-20.12	-18.18 CO2
Dolomite(disordered)	-0.23	-16.45	-16.22 CaMg(CO3)2
Dolomite(ordered)	0.37	-16.45	-16.81 CaMg(CO3)2
Epsomite	-3.60	-5.80	-2.21 MgSO4:7H2O
Fe(OH)2	-5.09	8.48	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	5.89	2.85	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-4.36	-2.80	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-11.49	-32.12	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-38.69	-40.74	-2.05 Fe2(SO4)3
Fe3(OH)8	0.11	20.33	20.22 Fe3(OH)8
FeMoO4	-4.03	-14.04	-10.01 FeMoO4
Ferrihydrite	2.22	5.93	3.70 Fe(OH)3
Ferroselite	-37.99	-56.91	-18.93 FeSe2
FeSe	-25.78	-36.80	-11.01 FeSe
Goethite	5.01	5.93	0.91 FeOOH
Gummite	-10.33	-2.09	8.24 UO3
Gypsum	-0.85	-5.46	-4.62 CaSO4:2H2O
H-Jarosite	-6.79	-17.28	-10.49 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-9.30	-22.52	-13.22 H2MoO4
H2Se(g)	-40.42	-45.28	-4.85 H2Se
Halite	-7.06	-5.49	1.58 NaCl
Hausmannite	-14.42	49.55	63.96 Mn3O4
Hematite	12.37	11.85	-0.52 Fe2O3
Huntite	-4.02	-33.24	-29.22 CaMg3(CO3)4
Hydromagnesite	-14.60	-21.85	-7.24 Mg5(CO3)4(OH)2:4H2O
K-Jarosite	-0.06	-13.95	-13.89 KFe3(SO4)2(OH)6
K2MoO4	-19.15	-15.86	3.29 K2MoO4
K2SeO4	-19.82	-20.55	-0.73 K2SeO4
Lepidocrocite	4.56	5.93	1.37 FeOOH

Lime	-21.98	12.07	34.05	CaO
Maghemite	5.47	11.85	6.39	Fe ₂ O ₃
Magnesioferrite	4.78	23.58	18.80	Fe ₂ MgO ₄
Magnesite	-0.79	-8.39	-7.60	MgCO ₃
Magnetite	15.48	20.33	4.86	Fe ₃ O ₄
Manganite	-4.63	20.71	25.34	MnOOH
Melanterite	-6.70	-9.05	-2.35	FeSO ₄ ·7H ₂ O
Mg(OH) ₂ (active)	-7.07	11.73	18.79	Mg(OH) ₂
MgMoO ₄	-8.94	-10.79	-1.85	MgMoO ₄
MgSeO ₃ ·6H ₂ O	-5.95	-2.93	3.02	MgSeO ₃ ·6H ₂ O
MgSeO ₄ ·6H ₂ O	-14.28	-15.48	-1.20	MgSeO ₄ ·6H ₂ O
Mirabilite	-6.32	-7.99	-1.67	Na ₂ SO ₄ ·10H ₂ O
Mn ₂ (SO ₄) ₃	-58.80	-63.37	-4.57	Mn ₂ (SO ₄) ₃
MnCl ₂ ·4H ₂ O	-15.18	-12.39	2.79	MnCl ₂ ·4H ₂ O
MnSe	-41.33	-37.15	4.18	MnSe
MnSeO ₃	-7.66	-6.53	1.13	MnSeO ₃
MnSeO ₃ ·2H ₂ O	-7.45	-6.53	0.92	MnSeO ₃ ·2H ₂ O
MnSeO ₄ ·5H ₂ O	-17.03	-19.08	-2.05	MnSeO ₄ ·5H ₂ O
MnSO ₄	-12.44	-9.40	3.03	MnSO ₄
MoO ₃	-14.52	-22.52	-8.00	MoO ₃
Na-Jarosite	-2.36	-12.51	-10.15	NaFe ₃ (SO ₄) ₂ (OH) ₆
Na ₂ Mo ₂ O ₇	-18.50	-35.49	-16.99	Na ₂ Mo ₂ O ₇
Na ₂ MoO ₄	-14.53	-12.97	1.56	Na ₂ MoO ₄
Na ₂ MoO ₄ ·2H ₂ O	-14.20	-12.97	1.22	Na ₂ MoO ₄ ·2H ₂ O
Na ₂ SeO ₃ ·5H ₂ O	-15.41	-5.11	10.30	Na ₂ SeO ₃ ·5H ₂ O
Na ₂ SeO ₄	-18.94	-17.66	1.28	Na ₂ SeO ₄
Natron	-8.81	-10.58	-1.77	Na ₂ CO ₃ ·10H ₂ O
Nesquehonite	-3.89	-8.39	-4.50	MgCO ₃ ·3H ₂ O
Nsutite	-10.32	7.19	17.50	MnO ₂
O ₂ (g)	-36.75	50.32	87.07	O ₂
Periclase	-10.91	11.73	22.64	MgO
Portlandite	-11.63	12.07	23.70	Ca(OH) ₂
Pyrochroite	-7.74	8.13	15.87	Mn(OH) ₂
Pyrolusite	-9.99	33.29	43.27	MnO ₂
Rhodochrosite	-1.43	-11.99	-10.57	MnCO ₃
Rutherfordine	-7.73	-22.21	-14.48	UO ₂ CO ₃
Schoepite	-8.43	-2.09	6.34	UO ₂ (OH) ₂ ·H ₂ O
Semetal(am)	-12.93	-20.12	-7.19	Se
Semetal(hex)	-12.30	-20.12	-7.82	Se
SeO ₂	-14.77	-14.66	0.11	SeO ₂
SeO ₃	-49.27	-27.21	22.06	SeO ₃
Siderite	-1.51	-11.64	-10.13	FeCO ₃
Thenardite	-8.37	-7.98	0.39	Na ₂ SO ₄
Thermonatrite	-11.29	-10.58	0.71	Na ₂ CO ₃ ·H ₂ O
U ₃ O ₈	-25.23	-0.77	24.46	U ₃ O ₈
U ₄ O ₉	-42.91	-42.96	-0.05	U ₄ O ₉
UO ₂ (am)	-18.73	-17.03	1.70	UO ₂
UO ₂ (NO ₃) ₂	-37.30	-24.57	12.73	UO ₂ (NO ₃) ₂
UO ₂ (NO ₃) ₂ ·2H ₂ O	-29.60	-24.57	5.03	UO ₂ (NO ₃) ₂ ·2H ₂ O
UO ₂ (NO ₃) ₂ ·3H ₂ O	-28.03	-24.57	3.45	UO ₂ (NO ₃) ₂ ·3H ₂ O
UO ₂ (NO ₃) ₂ ·6H ₂ O	-26.47	-24.57	1.90	UO ₂ (NO ₃) ₂ ·6H ₂ O
UO ₂ (OH) ₂ (beta)	-8.10	-2.09	6.01	UO ₂ (OH) ₂
UO ₂ SeO ₄ ·4H ₂ O	-27.05	-29.30	-2.25	UO ₂ SeO ₄ ·4H ₂ O
UO ₃	-10.35	-2.09	8.26	UO ₃
Uraninite	-12.90	-17.03	-4.13	UO ₂

**For a gas, SI = log₁₀(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 20. SAG2-3

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

Elements	Molality	Moles
Alkalinity	4.981e-03	4.981e-03

Ca	4.046e-03	4.046e-03
Cl	1.607e-03	1.607e-03
Fe(2)	5.323e-05	5.323e-05
Fe(3)	4.660e-06	4.660e-06
K	1.116e-04	1.116e-04
Mg	1.923e-03	1.923e-03
Mn	1.592e-05	1.592e-05
Mo	1.043e-07	1.043e-07
N(-3)	2.709e-05	2.709e-05
N(5)	1.429e-06	1.429e-06
Na	3.083e-03	3.083e-03
O(0)	3.316e-05	3.316e-05
S(-2)	1.998e-06	1.998e-06
S(6)	4.137e-03	4.137e-03
Se	6.465e-09	6.465e-09
U	2.620e-08	2.620e-08

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

pH = 7.440
 pe = 1.000
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.095e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 5.352e-03
 Total CO2 (mol/kg) = 5.352e-03
 Temperature (°C) = 13.70
 Electrical balance (eq) = 4.413e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.71
 Iterations = 17 (343 overall)
 Total H = 1.110195e+02
 Total O = 5.553948e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	2.2799	0.1298
N(-3)/N(5)	6.1017	0.3473
O(-2)/O(0)	13.6943	0.7794
S(-2)/S(6)	-3.7096	-0.2111

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	1.318e-07	1.142e-07	-6.880	-6.942	-0.062	(0)	
H+	4.170e-08	3.631e-08	-7.380	-7.440	-0.060	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	
C(4)	5.352e-03						
HCO3-	4.766e-03	4.173e-03	-2.322	-2.380	-0.058	(0)	
H2CO3	3.942e-04	3.942e-04	-3.404	-3.404	0.000	(0)	
CaHCO3+	1.196e-04	1.050e-04	-3.922	-3.979	-0.056	(0)	
MgHCO3+	4.247e-05	3.691e-05	-4.372	-4.433	-0.061	(0)	
CaCO3	9.753e-06	9.753e-06	-5.011	-5.011	0.000	(0)	
NaHCO3	7.740e-06	7.740e-06	-5.111	-5.111	0.000	(0)	
CO3-2	7.436e-06	4.273e-06	-5.129	-5.369	-0.241	(0)	
MgCO3	2.705e-06	2.705e-06	-5.568	-5.568	0.000	(0)	
FeHCO3+	1.056e-06	9.269e-07	-5.977	-6.033	-0.056	(0)	
MnHCO3+	6.138e-07	5.363e-07	-6.212	-6.271	-0.059	(0)	
NaCO3-	3.330e-07	2.915e-07	-6.478	-6.535	-0.058	(0)	
Ca2UO2(CO3)3	2.026e-08	2.036e-08	-7.693	-7.691	0.002	(0)	
CaUO2(CO3)3-2	5.761e-09	3.310e-09	-8.240	-8.480	-0.241	(0)	
UO2(CO3)3-4	1.278e-10	8.852e-12	-9.894	-11.053	-1.159	(0)	
UO2(CO3)2-2	3.309e-11	1.698e-11	-10.480	-10.770	-0.290	(0)	

MgUO2(CO3)3-2 1.976e-11 1.136e-11 -10.704 -10.945 -0.241 (0)
UO2CO3 2.410e-13 2.410e-13 -12.618 -12.618 0.000 (0)
(UO2)2CO3(OH)3- 3.759e-18 3.273e-18 -17.425 -17.485 -0.060 (0)
(UO2)3(CO3)6-6 1.012e-26 6.907e-29 -25.995 -28.161 -2.166 (0)
Ca 4.046e-03
Ca+2 3.232e-03 1.857e-03 -2.491 -2.731 -0.241 (0)
CaSO4 6.847e-04 6.847e-04 -3.164 -3.164 0.000 (0)
CaHCO3+ 1.196e-04 1.050e-04 -3.922 -3.979 -0.056 (0)
CaCO3 9.753e-06 9.753e-06 -5.011 -5.011 0.000 (0)
Ca2UO2(CO3)3 2.026e-08 2.036e-08 -7.693 -7.691 0.002 (0)
CaNO3+ 9.347e-09 7.911e-09 -8.029 -8.102 -0.072 (0)
CaUO2(CO3)3-2 5.761e-09 3.310e-09 -8.240 -8.480 -0.241 (0)
CaOH+ 4.224e-09 3.709e-09 -8.374 -8.431 -0.056 (0)
CaNH3+2 1.629e-09 8.357e-10 -8.788 -9.078 -0.290 (0)
Ca(NH3)2+2 2.318e-16 1.189e-16 -15.635 -15.925 -0.290 (0)
Cl 1.607e-03
Cl- 1.607e-03 1.399e-03 -2.794 -2.854 -0.060 (0)
MnCl+ 1.383e-08 1.209e-08 -7.859 -7.918 -0.059 (0)
MnCl2 2.388e-11 2.388e-11 -10.622 -10.622 0.000 (0)
MnCl3- 1.053e-14 9.200e-15 -13.978 -14.036 -0.059 (0)
FeCl+2 1.005e-17 5.856e-18 -16.998 -17.232 -0.234 (0)
FeCl2+ 6.034e-20 5.273e-20 -19.219 -19.278 -0.059 (0)
UO2Cl+ 3.138e-20 2.656e-20 -19.503 -19.576 -0.072 (0)
FeCl3 7.375e-24 7.375e-24 -23.132 -23.132 0.000 (0)
UO2Cl2 2.203e-24 2.213e-24 -23.657 -23.655 0.002 (0)
UCl+3 1.843e-39 4.106e-40 -38.734 -39.387 -0.652 (0)
Fe(2) 5.323e-05
Fe+2 4.337e-05 2.225e-05 -4.363 -4.653 -0.290 (0)
FeSO4 8.666e-06 8.666e-06 -5.062 -5.062 0.000 (0)
FeHCO3+ 1.056e-06 9.269e-07 -5.977 -6.033 -0.056 (0)
FeOH+ 1.158e-07 1.012e-07 -6.936 -6.995 -0.059 (0)
Fe(HS)2 2.474e-08 2.474e-08 -7.607 -7.607 0.000 (0)
Fe(OH)2 8.082e-12 8.082e-12 -11.092 -11.092 0.000 (0)
Fe(HS)3- 3.556e-12 3.009e-12 -11.449 -11.522 -0.072 (0)
Fe(OH)3- 7.278e-13 6.359e-13 -12.138 -12.197 -0.059 (0)
Fe(3) 4.660e-06
Fe(OH)2+ 4.406e-06 3.857e-06 -5.356 -5.414 -0.058 (0)
Fe(OH)3 2.207e-07 2.207e-07 -6.656 -6.656 0.000 (0)
Fe(OH)4- 3.386e-08 2.965e-08 -7.470 -7.528 -0.058 (0)
FeOH+2 3.157e-11 1.840e-11 -10.501 -10.735 -0.234 (0)
FeSO4+ 3.107e-15 2.715e-15 -14.508 -14.566 -0.059 (0)
Fe+3 6.950e-16 1.998e-16 -15.158 -15.699 -0.541 (0)
Fe(SO4)2- 1.355e-16 1.147e-16 -15.868 -15.941 -0.072 (0)
FeCl+2 1.005e-17 5.856e-18 -16.998 -17.232 -0.234 (0)
Fe2(OH)2+4 2.447e-19 1.695e-20 -18.611 -19.771 -1.159 (0)
FeCl2+ 6.034e-20 5.273e-20 -19.219 -19.278 -0.059 (0)
FeNO3+2 8.667e-21 4.447e-21 -20.062 -20.352 -0.290 (0)
FeHSeO3+2 3.243e-21 1.664e-21 -20.489 -20.779 -0.290 (0)
Fe3(OH)4+5 5.427e-23 8.373e-25 -22.265 -24.077 -1.812 (0)
FeCl3 7.375e-24 7.375e-24 -23.132 -23.132 0.000 (0)
H(0) 2.088e-20
H2 1.044e-20 1.049e-20 -19.981 -19.979 0.002 (0)
K 1.116e-04
K+ 1.103e-04 9.604e-05 -3.957 -4.018 -0.060 (0)
KSO4- 1.311e-06 1.148e-06 -5.882 -5.940 -0.058 (0)
Mg 1.923e-03
Mg+2 1.603e-03 9.210e-04 -2.795 -3.036 -0.241 (0)
MgSO4 2.753e-04 2.753e-04 -3.560 -3.560 0.000 (0)
MgHCO3+ 4.247e-05 3.691e-05 -4.372 -4.433 -0.061 (0)
MgCO3 2.705e-06 2.705e-06 -5.568 -5.568 0.000 (0)
MgOH+ 3.931e-08 3.460e-08 -7.405 -7.461 -0.055 (0)
MgUO2(CO3)3-2 1.976e-11 1.136e-11 -10.704 -10.945 -0.241 (0)
Mn(2) 1.592e-05
Mn+2 1.338e-05 6.864e-06 -4.874 -5.163 -0.290 (0)
MnSO4 1.915e-06 1.915e-06 -5.718 -5.718 0.000 (0)
MnHCO3+ 6.138e-07 5.363e-07 -6.212 -6.271 -0.059 (0)

MnCl+	1.383e-08	1.209e-08	-7.859	-7.918	-0.059	(0)
MnOH+	2.254e-09	1.969e-09	-8.647	-8.706	-0.059	(0)
MnCl2	2.388e-11	2.388e-11	-10.622	-10.622	0.000	(0)
MnNO3+	1.589e-11	1.345e-11	-10.799	-10.871	-0.072	(0)
MnCl3-	1.053e-14	9.200e-15	-13.978	-14.036	-0.059	(0)
Mn(NO3)2	4.288e-17	4.288e-17	-16.368	-16.368	0.000	(0)
MnSe	6.068e-18	6.068e-18	-17.217	-17.217	0.000	(0)
Mn(OH)3-	2.599e-18	2.271e-18	-17.585	-17.644	-0.059	(0)
Mn(OH)4-2	3.487e-24	2.032e-24	-23.458	-23.692	-0.234	(0)
MnSeO4	2.913e-25	2.913e-25	-24.536	-24.536	0.000	(0)
Mn(3)	1.923e-30					
Mn+3	1.923e-30	5.529e-31	-29.716	-30.257	-0.541	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-64.739	-64.973	-0.234	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-74.052	-74.115	-0.063	(0)
Mo	1.043e-07					
MoO4-2	1.043e-07	5.993e-08	-6.982	-7.222	-0.241	(0)
HMoO4-	3.723e-11	3.151e-11	-10.429	-10.502	-0.072	(0)
H2MoO4	1.741e-14	1.741e-14	-13.759	-13.759	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-52.904	-55.512	-2.609	(0)
HMo7O24-5	0.000e+00	0.000e+00	-54.823	-56.635	-1.812	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-58.154	-59.313	-1.159	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-62.841	-63.493	-0.652	(0)
N(-3)	2.709e-05					
NH4+	2.642e-05	2.276e-05	-4.578	-4.643	-0.065	(0)
NH4SO4-	5.029e-07	4.394e-07	-6.299	-6.357	-0.059	(0)
NH3	1.564e-07	1.564e-07	-6.806	-6.806	0.000	(0)
CaNH3+2	1.629e-09	8.357e-10	-8.788	-9.078	-0.290	(0)
Ca(NH3)2+2	2.318e-16	1.189e-16	-15.635	-15.925	-0.290	(0)
N(5)	1.429e-06					
NO3-	1.420e-06	1.236e-06	-5.848	-5.908	-0.060	(0)
CaNO3+	9.347e-09	7.911e-09	-8.029	-8.102	-0.072	(0)
MnNO3+	1.589e-11	1.345e-11	-10.799	-10.871	-0.072	(0)
Mn(NO3)2	4.288e-17	4.288e-17	-16.368	-16.368	0.000	(0)
FeNO3+2	8.667e-21	4.447e-21	-20.062	-20.352	-0.290	(0)
UO2NO3+	5.325e-23	4.506e-23	-22.274	-22.346	-0.072	(0)
Na	3.083e-03					
Na+	3.046e-03	2.652e-03	-2.516	-2.576	-0.060	(0)
NaSO4-	2.884e-05	2.525e-05	-4.540	-4.598	-0.058	(0)
NaHCO3	7.740e-06	7.740e-06	-5.111	-5.111	0.000	(0)
NaCO3-	3.330e-07	2.915e-07	-6.478	-6.535	-0.058	(0)
O(0)	3.316e-05					
O2	1.658e-05	1.666e-05	-4.780	-4.778	0.002	(0)
S(-2)	1.998e-06					
HS-	1.320e-06	1.117e-06	-5.879	-5.952	-0.072	(0)
H2S	6.024e-07	6.024e-07	-6.220	-6.220	0.000	(0)
Fe(HS)2	2.474e-08	2.474e-08	-7.607	-7.607	0.000	(0)
S5-2	1.423e-08	7.302e-09	-7.847	-8.137	-0.290	(0)
S6-2	7.887e-09	4.046e-09	-8.103	-8.393	-0.290	(0)
S4-2	3.515e-09	1.803e-09	-8.454	-8.744	-0.290	(0)
S3-2	5.248e-10	2.692e-10	-9.280	-9.570	-0.290	(0)
S2-2	4.730e-11	2.427e-11	-10.325	-10.615	-0.290	(0)
Fe(HS)3-	3.556e-12	3.009e-12	-11.449	-11.522	-0.072	(0)
S-2	1.207e-16	7.033e-17	-15.918	-16.153	-0.234	(0)
S(6)	4.137e-03					
SO4-2	3.135e-03	1.802e-03	-2.504	-2.744	-0.241	(0)
CaSO4	6.847e-04	6.847e-04	-3.164	-3.164	0.000	(0)
MgSO4	2.753e-04	2.753e-04	-3.560	-3.560	0.000	(0)
NaSO4-	2.884e-05	2.525e-05	-4.540	-4.598	-0.058	(0)
FeSO4	8.666e-06	8.666e-06	-5.062	-5.062	0.000	(0)
MnSO4	1.915e-06	1.915e-06	-5.718	-5.718	0.000	(0)
KSO4-	1.311e-06	1.148e-06	-5.882	-5.940	-0.058	(0)
NH4SO4-	5.029e-07	4.394e-07	-6.299	-6.357	-0.059	(0)
HSO4-	5.171e-09	4.506e-09	-8.286	-8.346	-0.060	(0)
FeSO4+	3.107e-15	2.715e-15	-14.508	-14.566	-0.059	(0)

Fe(SO4)2-	1.355e-16	1.147e-16	-15.868	-15.941	-0.072	(0)
UO2SO4	2.996e-17	2.996e-17	-16.523	-16.523	0.000	(0)
UO2(SO4)2-2	1.042e-18	5.345e-19	-17.982	-18.272	-0.290	(0)
U(SO4)2	2.590e-34	2.590e-34	-33.587	-33.587	0.000	(0)
USO4+2	5.248e-35	2.692e-35	-34.280	-34.570	-0.290	(0)
Se(-2)	9.211e-15					
HSe-	9.203e-15	7.789e-15	-14.036	-14.109	-0.072	(0)
MnSe	6.068e-18	6.068e-18	-17.217	-17.217	0.000	(0)
H2Se	2.083e-18	2.083e-18	-17.681	-17.681	0.000	(0)
Se-2	1.947e-22	9.986e-23	-21.711	-22.001	-0.290	(0)
Se(4)	6.465e-09					
HSeO3-	5.540e-09	4.689e-09	-8.256	-8.329	-0.072	(0)
SeO3-2	9.253e-10	4.747e-10	-9.034	-9.324	-0.290	(0)
H2SeO3	6.581e-14	6.581e-14	-13.182	-13.182	0.000	(0)
FeHSeO3+2	3.243e-21	1.664e-21	-20.489	-20.779	-0.290	(0)
Se(6)	3.431e-22					
SeO4-2	3.428e-22	1.970e-22	-21.465	-21.706	-0.241	(0)
MnSeO4	2.913e-25	2.913e-25	-24.536	-24.536	0.000	(0)
HSeO4-	2.938e-28	2.487e-28	-27.532	-27.604	-0.072	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-48.219	-48.871	-0.652	(0)
U(4)	9.679e-16					
U(OH)5-	9.664e-16	8.179e-16	-15.015	-15.087	-0.072	(0)
U(OH)4	1.500e-18	1.500e-18	-17.824	-17.824	0.000	(0)
U(OH)3+	2.709e-22	2.293e-22	-21.567	-21.640	-0.072	(0)
U(OH)2+2	1.041e-26	5.338e-27	-25.983	-26.273	-0.290	(0)
UOH+3	6.234e-32	1.389e-32	-31.205	-31.857	-0.652	(0)
U(SO4)2	2.590e-34	2.590e-34	-33.587	-33.587	0.000	(0)
USO4+2	5.248e-35	2.692e-35	-34.280	-34.570	-0.290	(0)
U+4	6.153e-38	4.262e-39	-37.211	-38.370	-1.159	(0)
UCl+3	1.843e-39	4.106e-40	-38.734	-39.387	-0.652	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-129.910	-135.779	-5.870	(0)
U(5)	1.354e-15					
UO2+	1.354e-15	1.146e-15	-14.868	-14.941	-0.072	(0)
U(6)	2.620e-08					
Ca2UO2(CO3)3	2.026e-08	2.036e-08	-7.693	-7.691	0.002	(0)
CaUO2(CO3)3-2	5.761e-09	3.310e-09	-8.240	-8.480	-0.241	(0)
UO2(CO3)3-4	1.278e-10	8.852e-12	-9.894	-11.053	-1.159	(0)
UO2(CO3)2-2	3.309e-11	1.698e-11	-10.480	-10.770	-0.290	(0)
MgUO2(CO3)3-2	1.976e-11	1.136e-11	-10.704	-10.945	-0.241	(0)
UO2(OH)2	5.520e-13	5.546e-13	-12.258	-12.256	0.002	(0)
UO2CO3	2.410e-13	2.410e-13	-12.618	-12.618	0.000	(0)
UO2(OH)3-	2.172e-14	1.891e-14	-13.663	-13.723	-0.060	(0)
UO2OH+	2.913e-16	2.465e-16	-15.536	-15.608	-0.072	(0)
UO2SO4	2.996e-17	2.996e-17	-16.523	-16.523	0.000	(0)
UO2+2	2.627e-17	1.510e-17	-16.580	-16.821	-0.241	(0)
(UO2)2CO3(OH)3-	3.759e-18	3.273e-18	-17.425	-17.485	-0.060	(0)
UO2(SO4)2-2	1.042e-18	5.345e-19	-17.982	-18.272	-0.290	(0)
UO2Cl+	3.138e-20	2.656e-20	-19.503	-19.576	-0.072	(0)
UO2(OH)4-2	1.412e-20	8.114e-21	-19.850	-20.091	-0.241	(0)
UO2NO3+	5.325e-23	4.506e-23	-22.274	-22.346	-0.072	(0)
UO2Cl2	2.203e-24	2.213e-24	-23.657	-23.655	0.002	(0)
(UO2)2(OH)2+2	4.621e-25	2.371e-25	-24.335	-24.625	-0.290	(0)
(UO2)3(CO3)6-6	1.012e-26	6.907e-29	-25.995	-28.161	-2.166	(0)
(UO2)2OH+3	4.284e-29	1.232e-29	-28.368	-28.910	-0.541	(0)
(UO2)3(OH)7-	4.217e-30	3.672e-30	-29.375	-29.435	-0.060	(0)
(UO2)3(OH)5+	3.004e-30	2.543e-30	-29.522	-29.595	-0.072	(0)
(UO2)3(OH)4+2	4.053e-33	2.329e-33	-32.392	-32.633	-0.241	(0)
(UO2)4(OH)7+	8.016e-38	6.979e-38	-37.096	-37.156	-0.060	(0)

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

Phase SI** log IAP log K(286 K, 1 atm)

(NH4)2SeO4 -31.44 -30.99 0.45 (NH4)2SeO4
 Anhydrite -1.17 -5.48 -4.31 CaSO4

Aragonite	0.12	-8.10	-8.22	CaCO ₃
Artinite	-6.99	3.44	10.43	MgCO ₃ :Mg(OH) ₂ :3H ₂ O
Birnessite	-17.59	0.50	18.09	MnO ₂
Bixbyite	-16.09	-15.88	0.21	Mn ₂ O ₃
Brucite	-5.79	11.84	17.63	Mg(OH) ₂
Calcite	0.32	-8.10	-8.42	CaCO ₃
CaMoO ₄	-2.02	-9.95	-7.94	CaMoO ₄
CaSeO ₃ :2H ₂ O	-6.57	-3.62	2.95	CaSeO ₃ :2H ₂ O
CaSeO ₄ :2H ₂ O	-21.47	-24.44	-2.96	CaSeO ₄ :2H ₂ O
CH ₄ (g)	-44.95	-87.77	-42.82	CH ₄
CO ₂ (g)	-2.07	-20.25	-18.18	CO ₂
Dolomite(disordered)	-0.29	-16.51	-16.22	CaMg(CO ₃) ₂
Dolomite(ordered)	0.31	-16.51	-16.82	CaMg(CO ₃) ₂
Epsomite	-3.57	-5.78	-2.21	MgSO ₄ :7H ₂ O
Fe(OH) ₂	-3.34	10.23	13.56	Fe(OH) ₂
Fe(OH) ₂ .7Cl ₃	6.57	3.53	-3.04	Fe(OH) ₂ .7Cl ₃
Fe ₂ (OH) ₄ SeO ₃	-4.08	-2.53	1.55	Fe ₂ (OH) ₄ SeO ₃
Fe ₂ (SeO ₃) ₃ :2H ₂ O	-13.44	-34.07	-20.63	Fe ₂ (SeO ₃) ₃ :2H ₂ O
Fe ₂ (SO ₄) ₃	-37.57	-39.63	-2.06	Fe ₂ (SO ₄) ₃
Fe ₃ (OH) ₈	3.25	23.47	20.22	Fe ₃ (OH) ₈
FeMoO ₄	-1.86	-11.88	-10.01	FeMoO ₄
Ferrihydrite	2.92	6.62	3.70	Fe(OH) ₃
Ferroselite	2.93	-15.99	-18.92	FeSe ₂
FeS(ppt)	-0.29	-3.16	-2.87	FeS
FeSe	-0.31	-11.32	-11.01	FeSe
Goethite	5.71	6.62	0.91	FeOOH
Greigite	14.94	-30.10	-45.03	Fe ₃ S ₄
Gummite	-10.17	-1.94	8.23	UO ₃
Gypsum	-0.86	-5.48	-4.62	CaSO ₄ :2H ₂ O
H-Jarosite	-4.88	-15.39	-10.51	(H ₃ O)Fe ₃ (SO ₄) ₂ (OH) ₆
H ₂ MoO ₄	-8.89	-22.10	-13.21	H ₂ MoO ₄
H ₂ S(g)	-5.38	-13.39	-8.01	H ₂ S
H ₂ Se(g)	-16.69	-21.55	-4.85	H ₂ Se
Halite	-7.01	-5.43	1.58	NaCl
Hausmannite	-17.91	46.03	63.94	Mn ₃ O ₄
Hematite	13.77	13.24	-0.53	Fe ₂ O ₃
Huntite	-4.09	-33.32	-29.22	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-14.52	-21.78	-7.26	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
K-Jarosite	1.93	-11.97	-13.90	KFe ₃ (SO ₄) ₂ (OH) ₆
K ₂ MoO ₄	-18.54	-15.26	3.29	K ₂ MoO ₄
K ₂ SeO ₄	-29.01	-29.74	-0.73	K ₂ SeO ₄
Lepidocrocite	5.25	6.62	1.37	FeOOH
Lime	-21.89	12.15	34.04	CaO
Mackinawite	0.44	-3.16	-3.60	FeS
Maghemite	6.85	13.24	6.39	Fe ₂ O ₃
Magnesianoferrite	6.30	25.08	18.78	Fe ₂ MgO ₄
Magnesite	-0.81	-8.41	-7.60	MgCO ₃
Magnetite	18.63	23.47	4.84	Fe ₃ O ₄
Manganite	-7.18	18.16	25.34	MnOOH
Melanterite	-5.05	-7.40	-2.35	FeSO ₄ :7H ₂ O
Mg(OH) ₂ (active)	-6.95	11.84	18.79	Mg(OH) ₂
MgMoO ₄	-8.41	-10.26	-1.85	MgMoO ₄
MgSeO ₃ :6H ₂ O	-6.94	-3.93	3.02	MgSeO ₃ :6H ₂ O
MgSeO ₄ :6H ₂ O	-23.54	-24.74	-1.20	MgSeO ₄ :6H ₂ O
Mirabilite	-6.24	-7.90	-1.66	Na ₂ SO ₄ :10H ₂ O
Mn ₂ (SO ₄) ₃	-64.16	-68.75	-4.58	Mn ₂ (SO ₄) ₃
MnCl ₂ :4H ₂ O	-13.66	-10.87	2.79	MnCl ₂ :4H ₂ O
MnS(grn)	-4.07	-3.68	0.39	MnS
MnS(pnk)	-7.02	-3.68	3.34	MnS
MnSe	-16.01	-11.83	4.18	MnSe
MnSeO ₃	-7.18	-6.05	1.13	MnSeO ₃
MnSeO ₃ :2H ₂ O	-6.98	-6.05	0.92	MnSeO ₃ :2H ₂ O
MnSeO ₄ :5H ₂ O	-24.82	-26.87	-2.05	MnSeO ₄ :5H ₂ O
MnSO ₄	-10.94	-7.91	3.03	MnSO ₄
MoO ₃	-14.10	-22.10	-8.00	MoO ₃
MoS ₂	7.18	-65.77	-72.94	MoS ₂

Na-Jarosite -0.37 -10.52 -10.16 NaFe3(SO4)2(OH)6
 Na2Mo2O7 -17.49 -34.48 -16.98 Na2Mo2O7
 Na2MoO4 -13.93 -12.38 1.56 Na2MoO4
 Na2MoO4:2H2O -13.60 -12.38 1.22 Na2MoO4:2H2O
 Na2SeO3:5H2O -16.34 -6.04 10.30 Na2SeO3:5H2O
 Na2SeO4 -28.14 -26.86 1.28 Na2SeO4
 Natron -8.76 -10.52 -1.77 Na2CO3:10H2O
 Nesquehonite -3.90 -8.41 -4.50 MgCO3:3H2O
 Nsutite -17.00 0.50 17.50 MnO2
 O2(g) -53.27 33.76 87.03 O2
 Periclase -10.78 11.84 22.63 MgO
 Portlandite -11.54 12.15 23.69 Ca(OH)2
 Pyrite 19.18 0.32 -18.85 FeS2
 Pyrochroite -6.15 9.72 15.86 Mn(OH)2
 Pyrolusite -16.66 26.60 43.26 MnO2
 Rhodochrosite 0.03 -10.53 -10.57 MnCO3
 Rutherfordine -7.71 -22.19 -14.48 UO2CO3
 Schoepite -8.28 -1.94 6.34 UO2(OH)2:H2O
 Semetal(am) 2.52 -4.67 -7.18 Se
 Semetal(hex) 3.15 -4.67 -7.82 Se
 SeO2 -15.88 -15.77 0.11 SeO2
 SeO3 -58.64 -36.59 22.05 SeO3
 Siderite 0.11 -10.02 -10.13 FeCO3
 Sulfur 5.52 3.49 -2.03 S
 Thenardite -8.28 -7.90 0.38 Na2SO4
 Thermonatrite -11.23 -10.52 0.71 Na2CO3:H2O
 U3O8 -16.51 7.93 24.43 U3O8
 U4O9 -17.49 -17.56 -0.07 U4O9
 UO2(am) -10.30 -8.61 1.69 UO2
 UO2(NO3)2 -41.36 -28.64 12.72 UO2(NO3)2
 UO2(NO3)2:2H2O -33.66 -28.64 5.03 UO2(NO3)2:2H2O
 UO2(NO3)2:3H2O -32.09 -28.64 3.45 UO2(NO3)2:3H2O
 UO2(NO3)2:6H2O -30.54 -28.64 1.90 UO2(NO3)2:6H2O
 UO2(OH)2(beta) -7.94 -1.94 6.00 UO2(OH)2
 UO2SeO4:4H2O -36.28 -38.53 -2.25 UO2SeO4:4H2O
 UO3 -10.20 -1.94 8.26 UO3
 Uraninite -4.48 -8.61 -4.13 UO2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

Initial solution 21. SAG2-4

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

Elements	Molality	Moles
Alkalinity	5.001e-03	5.001e-03
Ca	3.622e-03	3.622e-03
Cl	1.869e-03	1.869e-03
Fe(2)	8.245e-05	8.245e-05
Fe(3)	1.613e-06	1.613e-06
K	1.106e-04	1.106e-04
Mg	1.993e-03	1.993e-03
Mn	3.845e-05	3.845e-05
Mo	1.732e-07	1.732e-07
N(-3)	5.975e-05	5.975e-05
N(5)	1.429e-06	1.429e-06
Na	3.867e-03	3.867e-03
O(0)	1.752e-05	1.752e-05
S(6)	4.439e-03	4.439e-03
Se	1.268e-09	1.268e-09
U	1.556e-08	1.556e-08

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

pH = 7.750
 pe = 0.700
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.146e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 5.153e-03
 Total CO2 (mol/kg) = 5.153e-03
 Temperature (°C) = 13.60
 Electrical balance (eq) = -2.392e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.89
 Iterations = 15 (358 overall)
 Total H = 1.110192e+02
 Total O = 5.554007e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	0.9911	0.0564
N(-3)/N(5)	5.6779	0.3230
O(-2)/O(0)	13.3227	0.7580

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	2.673e-07	2.313e-07	-6.573	-6.636	-0.063	(0)	
H+	2.045e-08	1.778e-08	-7.689	-7.750	-0.061	0.00	
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03	
C(4)	5.153e-03						
HCO3-	4.761e-03	4.163e-03	-2.322	-2.381	-0.058	(0)	
H2CO3	1.928e-04	1.928e-04	-3.715	-3.715	0.000	(0)	
CaHCO3+	1.044e-04	9.158e-05	-3.981	-4.038	-0.057	(0)	
MgHCO3+	4.316e-05	3.746e-05	-4.365	-4.426	-0.062	(0)	
CaCO3	1.734e-05	1.734e-05	-4.761	-4.761	0.000	(0)	
CO3-2	1.519e-05	8.684e-06	-4.818	-5.061	-0.243	(0)	
NaHCO3	9.683e-06	9.683e-06	-5.014	-5.014	0.000	(0)	
MgCO3	5.587e-06	5.587e-06	-5.253	-5.253	0.000	(0)	
FeHCO3+	1.594e-06	1.398e-06	-5.797	-5.854	-0.057	(0)	
MnHCO3+	1.455e-06	1.269e-06	-5.837	-5.896	-0.059	(0)	
NaCO3-	8.505e-07	7.437e-07	-6.070	-6.129	-0.058	(0)	
Ca2UO2(CO3)3	1.164e-08	1.170e-08	-7.934	-7.932	0.002	(0)	
CaUO2(CO3)3-2	3.796e-09	2.169e-09	-8.421	-8.664	-0.243	(0)	
UO2(CO3)3-4	9.919e-11	6.656e-12	-10.004	-11.177	-1.173	(0)	
MgUO2(CO3)3-2	1.512e-11	8.643e-12	-10.820	-11.063	-0.243	(0)	
UO2(CO3)2-2	1.224e-11	6.230e-12	-10.912	-11.206	-0.293	(0)	
UO2CO3	4.358e-14	4.358e-14	-13.361	-13.361	0.000	(0)	
(UO2)2CO3(OH)3-	5.173e-19	4.498e-19	-18.286	-18.347	-0.061	(0)	
(UO2)3(CO3)6-6	5.349e-28	3.481e-30	-27.272	-29.458	-2.187	(0)	
Ca	3.622e-03						
Ca+2	2.849e-03	1.628e-03	-2.545	-2.788	-0.243	(0)	
CaSO4	6.511e-04	6.511e-04	-3.186	-3.186	0.000	(0)	
CaHCO3+	1.044e-04	9.158e-05	-3.981	-4.038	-0.057	(0)	
CaCO3	1.734e-05	1.734e-05	-4.761	-4.761	0.000	(0)	
Ca2UO2(CO3)3	1.164e-08	1.170e-08	-7.934	-7.932	0.002	(0)	
CaNO3+	8.214e-09	6.938e-09	-8.085	-8.159	-0.073	(0)	
CaOH+	7.499e-09	6.577e-09	-8.125	-8.182	-0.057	(0)	
CaNH3+2	6.425e-09	3.270e-09	-8.192	-8.485	-0.293	(0)	
CaUO2(CO3)3-2	3.796e-09	2.169e-09	-8.421	-8.664	-0.243	(0)	
Ca(NH3)2+2	4.080e-15	2.077e-15	-14.389	-14.683	-0.293	(0)	
Cl	1.869e-03						
Cl-	1.869e-03	1.625e-03	-2.728	-2.789	-0.061	(0)	
MnCl+	3.820e-08	3.334e-08	-7.418	-7.477	-0.059	(0)	
MnCl2	7.653e-11	7.653e-11	-10.116	-10.116	0.000	(0)	
MnCl3-	3.926e-14	3.426e-14	-13.406	-13.465	-0.059	(0)	

FeCl+2	9.058e-19	5.252e-19	-18.043	-18.280	-0.237	(0)
FeCl2+	6.318e-21	5.514e-21	-20.199	-20.259	-0.059	(0)
UO2Cl+	3.245e-21	2.741e-21	-20.489	-20.562	-0.073	(0)
FeCl3	8.961e-25	8.961e-25	-24.048	-24.048	0.000	(0)
UO2Cl2	2.647e-25	2.661e-25	-24.577	-24.575	0.002	(0)
UCl+3	0.000e+00	0.000e+00	-40.341	-41.001	-0.660	(0)
Fe(2)	8.245e-05					
Fe+2	6.626e-05	3.372e-05	-4.179	-4.472	-0.293	(0)
FeSO4	1.424e-05	1.424e-05	-4.846	-4.846	0.000	(0)
FeHCO3+	1.594e-06	1.398e-06	-5.797	-5.854	-0.057	(0)
FeOH+	3.558e-07	3.105e-07	-6.449	-6.508	-0.059	(0)
Fe(OH)2	5.018e-11	5.018e-11	-10.299	-10.299	0.000	(0)
Fe(OH)3-	9.228e-12	8.053e-12	-11.035	-11.094	-0.059	(0)
Fe(3)	1.613e-06					
Fe(OH)2+	1.424e-06	1.245e-06	-5.846	-5.905	-0.058	(0)
Fe(OH)3	1.433e-07	1.433e-07	-6.844	-6.844	0.000	(0)
Fe(OH)4-	4.564e-08	3.991e-08	-7.341	-7.399	-0.058	(0)
FeOH+2	4.988e-12	2.893e-12	-11.302	-11.539	-0.237	(0)
FeSO4+	2.607e-16	2.275e-16	-15.584	-15.643	-0.059	(0)
Fe+3	5.448e-17	1.547e-17	-16.264	-16.810	-0.547	(0)
Fe(SO4)2-	1.236e-17	1.044e-17	-16.908	-16.981	-0.073	(0)
FeCl+2	9.058e-19	5.252e-19	-18.043	-18.280	-0.237	(0)
FeCl2+	6.318e-21	5.514e-21	-20.199	-20.259	-0.059	(0)
Fe2(OH)2+4	6.265e-21	4.204e-22	-20.203	-21.376	-1.173	(0)
FeNO3+2	6.800e-22	3.461e-22	-21.167	-21.461	-0.293	(0)
FeHSeO3+2	4.291e-23	2.184e-23	-22.367	-22.661	-0.293	(0)
FeCl3	8.961e-25	8.961e-25	-24.048	-24.048	0.000	(0)
Fe3(OH)4+5	4.562e-25	6.697e-27	-24.341	-26.174	-1.833	(0)
H(0)	1.996e-20					
H2	9.980e-21	1.003e-20	-20.001	-19.999	0.002	(0)
K	1.106e-04					
K+	1.092e-04	9.495e-05	-3.962	-4.023	-0.061	(0)
KSO4-	1.408e-06	1.231e-06	-5.851	-5.910	-0.058	(0)
Mg	1.993e-03					
Mg+2	1.640e-03	9.376e-04	-2.785	-3.028	-0.243	(0)
MgSO4	3.041e-04	3.041e-04	-3.517	-3.517	0.000	(0)
MgHCO3+	4.316e-05	3.746e-05	-4.365	-4.426	-0.062	(0)
MgCO3	5.587e-06	5.587e-06	-5.253	-5.253	0.000	(0)
MgOH+	8.101e-08	7.122e-08	-7.091	-7.147	-0.056	(0)
MgUO2(CO3)3-2	1.512e-11	8.643e-12	-10.820	-11.063	-0.243	(0)
Mn(2)	3.845e-05					
Mn+2	3.201e-05	1.629e-05	-4.495	-4.788	-0.293	(0)
MnSO4	4.930e-06	4.930e-06	-5.307	-5.307	0.000	(0)
MnHCO3+	1.455e-06	1.269e-06	-5.837	-5.896	-0.059	(0)
MnCl+	3.820e-08	3.334e-08	-7.418	-7.477	-0.059	(0)
MnOH+	1.085e-08	9.466e-09	-7.965	-8.024	-0.059	(0)
MnCl2	7.653e-11	7.653e-11	-10.116	-10.116	0.000	(0)
MnNO3+	3.778e-11	3.191e-11	-10.423	-10.496	-0.073	(0)
MnCl3-	3.926e-14	3.426e-14	-13.406	-13.465	-0.059	(0)
Mn(NO3)2	1.017e-16	1.017e-16	-15.993	-15.993	0.000	(0)
Mn(OH)3-	5.257e-17	4.587e-17	-16.279	-16.338	-0.059	(0)
MnSe	4.357e-18	4.357e-18	-17.361	-17.361	0.000	(0)
Mn(OH)4-2	1.446e-22	8.383e-23	-21.840	-22.077	-0.237	(0)
MnSeO4	2.436e-25	2.436e-25	-24.613	-24.613	0.000	(0)
Mn(3)	2.280e-30					
Mn+3	2.280e-30	6.475e-31	-29.642	-30.189	-0.547	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-63.126	-63.363	-0.237	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-72.748	-72.812	-0.064	(0)
Mo	1.732e-07					
MoO4-2	1.732e-07	9.898e-08	-6.762	-7.004	-0.243	(0)
HMoO4-	3.009e-11	2.541e-11	-10.522	-10.595	-0.073	(0)
H2MoO4	6.922e-15	6.922e-15	-14.160	-14.160	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-53.813	-56.453	-2.640	(0)
HMo7O24-5	0.000e+00	0.000e+00	-56.052	-57.886	-1.833	(0)

H2Mo7O24-4 0.000e+00 0.000e+00 -59.701 -60.874 -1.173 (0)
H3Mo7O24-3 0.000e+00 0.000e+00 -64.704 -65.364 -0.660 (0)
N(-3) 5.975e-05
NH4+ 5.785e-05 4.975e-05 -4.238 -4.303 -0.065 (0)
NH4SO4- 1.195e-06 1.043e-06 -5.923 -5.982 -0.059 (0)
NH3 6.929e-07 6.929e-07 -6.159 -6.159 0.000 (0)
CaNH3+2 6.425e-09 3.270e-09 -8.192 -8.485 -0.293 (0)
Ca(NH3)2+2 4.080e-15 2.077e-15 -14.389 -14.683 -0.293 (0)
N(5) 1.429e-06
NO3- 1.421e-06 1.236e-06 -5.847 -5.908 -0.061 (0)
CaNO3+ 8.214e-09 6.938e-09 -8.085 -8.159 -0.073 (0)
MnNO3+ 3.778e-11 3.191e-11 -10.423 -10.496 -0.073 (0)
Mn(NO3)2 1.017e-16 1.017e-16 -15.993 -15.993 0.000 (0)
FeNO3+2 6.800e-22 3.461e-22 -21.167 -21.461 -0.293 (0)
UO2NO3+ 4.756e-24 4.017e-24 -23.323 -23.396 -0.073 (0)
Na 3.867e-03
Na+ 3.817e-03 3.319e-03 -2.418 -2.479 -0.061 (0)
NaSO4- 3.924e-05 3.431e-05 -4.406 -4.465 -0.058 (0)
NaHCO3 9.683e-06 9.683e-06 -5.014 -5.014 0.000 (0)
NaCO3- 8.505e-07 7.437e-07 -6.070 -6.129 -0.058 (0)
O(0) 1.752e-05
O2 8.759e-06 8.802e-06 -5.058 -5.055 0.002 (0)
S(6) 4.439e-03
SO4-2 3.423e-03 1.956e-03 -2.466 -2.709 -0.243 (0)
CaSO4 6.511e-04 6.511e-04 -3.186 -3.186 0.000 (0)
MgSO4 3.041e-04 3.041e-04 -3.517 -3.517 0.000 (0)
NaSO4- 3.924e-05 3.431e-05 -4.406 -4.465 -0.058 (0)
FeSO4 1.424e-05 1.424e-05 -4.846 -4.846 0.000 (0)
MnSO4 4.930e-06 4.930e-06 -5.307 -5.307 0.000 (0)
KSO4- 1.408e-06 1.231e-06 -5.851 -5.910 -0.058 (0)
NH4SO4- 1.195e-06 1.043e-06 -5.923 -5.982 -0.059 (0)
HSO4- 2.745e-09 2.389e-09 -8.561 -8.622 -0.060 (0)
FeSO4+ 2.607e-16 2.275e-16 -15.584 -15.643 -0.059 (0)
Fe(SO4)2- 1.236e-17 1.044e-17 -16.908 -16.981 -0.073 (0)
UO2SO4 2.888e-18 2.888e-18 -17.539 -17.539 0.000 (0)
UO2(SO4)2-2 1.096e-19 5.580e-20 -18.960 -19.253 -0.293 (0)
U(SO4)2 6.330e-36 6.330e-36 -35.199 -35.199 0.000 (0)
USO4+2 1.195e-36 6.083e-37 -35.923 -36.216 -0.293 (0)
Se(-2) 1.371e-15
HSe- 1.366e-15 1.154e-15 -14.865 -14.938 -0.073 (0)
MnSe 4.357e-18 4.357e-18 -17.361 -17.361 0.000 (0)
H2Se 1.511e-19 1.511e-19 -18.821 -18.821 0.000 (0)
Se-2 5.893e-23 2.999e-23 -22.230 -22.523 -0.293 (0)
Se(4) 1.268e-09
HSeO3- 9.441e-10 7.975e-10 -9.025 -9.098 -0.073 (0)
SeO3-2 3.236e-10 1.647e-10 -9.490 -9.783 -0.293 (0)
H2SeO3 5.477e-15 5.477e-15 -14.261 -14.261 0.000 (0)
FeHSeO3+2 4.291e-23 2.184e-23 -22.367 -22.661 -0.293 (0)
Se(6) 1.219e-22
SeO4-2 1.217e-22 6.954e-23 -21.915 -22.158 -0.243 (0)
MnSeO4 2.436e-25 2.436e-25 -24.613 -24.613 0.000 (0)
HSeO4- 5.074e-29 4.286e-29 -28.295 -28.368 -0.073 (0)
U(3) 0.000e+00
U+3 0.000e+00 0.000e+00 -49.599 -50.259 -0.660 (0)
U(4) 7.043e-16
U(OH)5- 7.037e-16 5.944e-16 -15.153 -15.226 -0.073 (0)
U(OH)4 5.349e-19 5.349e-19 -18.272 -18.272 0.000 (0)
U(OH)3+ 4.747e-23 4.009e-23 -22.324 -22.397 -0.073 (0)
U(OH)2+2 9.010e-28 4.586e-28 -27.045 -27.339 -0.293 (0)
UOH+3 2.680e-33 5.865e-34 -32.572 -33.232 -0.660 (0)
U(SO4)2 6.330e-36 6.330e-36 -35.199 -35.199 0.000 (0)
USO4+2 1.195e-36 6.083e-37 -35.923 -36.216 -0.293 (0)
U+4 1.323e-39 0.000e+00 -38.878 -40.052 -1.173 (0)
UCl+3 0.000e+00 0.000e+00 -40.341 -41.001 -0.660 (0)
U6(OH)15+9 0.000e+00 0.000e+00 -135.277 -141.217 -5.940 (0)
U(5) 2.415e-16

UO2+ 2.415e-16 2.040e-16 -15.617 -15.690 -0.073 (0)
 U(6) 1.556e-08
 Ca2UO2(CO3)3 1.164e-08 1.170e-08 -7.934 -7.932 0.002 (0)
 CaUO2(CO3)3-2 3.796e-09 2.169e-09 -8.421 -8.664 -0.243 (0)
 UO2(CO3)3-4 9.919e-11 6.656e-12 -10.004 -11.177 -1.173 (0)
 MgUO2(CO3)3-2 1.512e-11 8.643e-12 -10.820 -11.063 -0.243 (0)
 UO2(CO3)2-2 1.224e-11 6.230e-12 -10.912 -11.206 -0.293 (0)
 UO2(OH)2 2.048e-13 2.059e-13 -12.689 -12.686 0.002 (0)
 UO2CO3 4.358e-14 4.358e-14 -13.361 -13.361 0.000 (0)
 UO2(OH)3- 1.648e-14 1.433e-14 -13.783 -13.844 -0.061 (0)
 UO2OH+ 5.268e-17 4.450e-17 -16.278 -16.352 -0.073 (0)
 UO2SO4 2.888e-18 2.888e-18 -17.539 -17.539 0.000 (0)
 UO2+2 2.352e-18 1.344e-18 -17.629 -17.872 -0.243 (0)
 (UO2)2CO3(OH)3- 5.173e-19 4.498e-19 -18.286 -18.347 -0.061 (0)
 UO2(SO4)2-2 1.096e-19 5.580e-20 -18.960 -19.253 -0.293 (0)
 UO2(OH)4-2 2.196e-20 1.255e-20 -19.658 -19.901 -0.243 (0)
 UO2Cl+ 3.245e-21 2.741e-21 -20.489 -20.562 -0.073 (0)
 UO2NO3+ 4.756e-24 4.017e-24 -23.323 -23.396 -0.073 (0)
 UO2Cl2 2.647e-25 2.661e-25 -24.577 -24.575 0.002 (0)
 (UO2)2(OH)2+2 1.530e-26 7.787e-27 -25.815 -26.109 -0.293 (0)
 (UO2)3(CO3)6-6 5.349e-28 3.481e-30 -27.272 -29.458 -2.187 (0)
 (UO2)2OH+3 7.018e-31 1.993e-31 -30.154 -30.700 -0.547 (0)
 (UO2)3(OH)7- 4.408e-31 3.833e-31 -30.356 -30.416 -0.061 (0)
 (UO2)3(OH)5+ 7.421e-32 6.268e-32 -31.130 -31.203 -0.073 (0)
 (UO2)3(OH)4+2 4.997e-35 2.856e-35 -34.301 -34.544 -0.243 (0)
 (UO2)4(OH)7+ 7.460e-40 6.487e-40 -39.127 -39.188 -0.061 (0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)
(NH4)2SeO4	-31.21	-30.76	0.45 (NH4)2SeO4
Anhydrite	-1.19	-5.50	-4.31 CaSO4
Aragonite	0.37	-7.85	-8.22 CaCO3
Artinite	-6.06	4.38	10.44 MgCO3:Mg(OH)2:3H2O
Birnessite	-16.58	1.51	18.09 MnO2
Bixbyite	-14.10	-13.88	0.22 Mn2O3
Brucite	-5.17	12.47	17.64 Mg(OH)2
Calcite	0.57	-7.85	-8.42 CaCO3
CaMoO4	-1.86	-9.79	-7.94 CaMoO4
CaSeO3:2H2O	-7.09	-4.14	2.95 CaSeO3:2H2O
CaSeO4:2H2O	-21.98	-24.95	-2.96 CaSeO4:2H2O
CH4(g)	-45.32	-88.16	-42.84 CH4
CO2(g)	-2.39	-20.56	-18.18 CO2
Dolomite(disordered)	0.28	-15.94	-16.22 CaMg(CO3)2
Dolomite(ordered)	0.88	-15.94	-16.81 CaMg(CO3)2
Epsomite	-3.53	-5.74	-2.21 MgSO4:7H2O
Fe(OH)2	-2.54	11.03	13.56 Fe(OH)2
Fe(OH)2.7Cl.3	6.32	3.28	-3.04 Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-5.52	-3.97	1.55 Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-17.04	-37.67	-20.63 Fe2(SeO3)3:2H2O
Fe2(SO4)3	-39.70	-41.75	-2.05 Fe2(SO4)3
Fe3(OH)8	3.68	23.91	20.22 Fe3(OH)8
FeMoO4	-1.46	-11.48	-10.01 FeMoO4
Ferrihydrite	2.74	6.44	3.70 Fe(OH)3
Ferroselite	1.48	-17.45	-18.93 FeSe2
FeSe	-0.65	-11.66	-11.01 FeSe
Goethite	5.53	6.44	0.91 FeOOH
Gummitite	-10.61	-2.37	8.24 UO3
Gypsum	-0.88	-5.50	-4.62 CaSO4:2H2O
H-Jarosite	-6.61	-17.10	-10.49 (H3O)Fe3(SO4)2(OH)6
H2MoO4	-9.29	-22.50	-13.22 H2MoO4
H2Se(g)	-17.83	-22.69	-4.85 H2Se
Halite	-6.84	-5.27	1.58 NaCl
Hausmannite	-14.93	49.04	63.96 Mn3O4
Hematite	13.40	12.88	-0.52 Fe2O3

Huntite	-2.90	-32.12	-29.22	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-12.64	-19.89	-7.24	Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O
K-Jarosite	0.52	-13.37	-13.89	KFe ₃ (SO ₄) ₂ (OH) ₆
K ₂ MoO ₄	-18.33	-15.05	3.29	K ₂ MoO ₄
K ₂ SeO ₄	-29.47	-30.20	-0.73	K ₂ SeO ₄
Lepidocrocite	5.07	6.44	1.37	FeOOH
Lime	-21.34	12.71	34.05	CaO
Maghemite	6.49	12.88	6.39	Fe ₂ O ₃
Magnesioferrite	6.55	25.35	18.80	Fe ₂ MgO ₄
Magnesite	-0.49	-8.09	-7.60	MgCO ₃
Magnetite	19.05	23.91	4.86	Fe ₃ O ₄
Manganite	-6.18	19.16	25.34	MnOOH
Melanterite	-4.83	-7.18	-2.35	FeSO ₄ ·7H ₂ O
Mg(OH) ₂ (active)	-6.32	12.47	18.79	Mg(OH) ₂
MgMoO ₄	-8.18	-10.03	-1.85	MgMoO ₄
MgSeO ₃ ·6H ₂ O	-7.40	-4.38	3.02	MgSeO ₃ ·6H ₂ O
MgSeO ₄ ·6H ₂ O	-23.99	-25.19	-1.20	MgSeO ₄ ·6H ₂ O
Mirabilite	-6.00	-7.67	-1.67	Na ₂ SO ₄ ·10H ₂ O
Mn ₂ (SO ₄) ₃	-63.93	-68.50	-4.57	Mn ₂ (SO ₄) ₃
MnCl ₂ ·4H ₂ O	-13.16	-10.37	2.79	MnCl ₂ ·4H ₂ O
MnSe	-16.16	-11.98	4.18	MnSe
MnSeO ₃	-7.27	-6.14	1.13	MnSeO ₃
MnSeO ₃ ·2H ₂ O	-7.06	-6.14	0.92	MnSeO ₃ ·2H ₂ O
MnSeO ₄ ·5H ₂ O	-24.90	-26.95	-2.05	MnSeO ₄ ·5H ₂ O
MnSO ₄	-10.53	-7.50	3.03	MnSO ₄
MoO ₃	-14.50	-22.50	-8.00	MoO ₃
Na-Jarosite	-1.68	-11.83	-10.15	NaFe ₃ (SO ₄) ₂ (OH) ₆
Na ₂ Mo ₂ O ₇	-17.48	-34.47	-16.99	Na ₂ Mo ₂ O ₇
Na ₂ MoO ₄	-13.52	-11.96	1.56	Na ₂ MoO ₄
Na ₂ MoO ₄ ·2H ₂ O	-13.19	-11.96	1.22	Na ₂ MoO ₄ ·2H ₂ O
Na ₂ SeO ₃ ·5H ₂ O	-16.61	-6.31	10.30	Na ₂ SeO ₃ ·5H ₂ O
Na ₂ SeO ₄	-28.40	-27.12	1.28	Na ₂ SeO ₄
Natron	-8.25	-10.02	-1.77	Na ₂ CO ₃ ·10H ₂ O
Nesquehonite	-3.59	-8.09	-4.50	MgCO ₃ ·3H ₂ O
Nsutite	-15.99	1.51	17.50	MnO ₂
O ₂ (g)	-53.27	33.80	87.07	O ₂
Periclase	-10.17	12.47	22.64	MgO
Portlandite	-10.99	12.71	23.70	Ca(OH) ₂
Pyrochroite	-5.16	10.71	15.87	Mn(OH) ₂
Pyrolusite	-15.66	27.61	43.27	MnO ₂
Rhodochrosite	0.72	-9.85	-10.57	MnCO ₃
Rutherfordine	-8.45	-22.93	-14.48	UO ₂ CO ₃
Schoepite	-8.71	-2.37	6.34	UO ₂ (OH) ₂ ·H ₂ O
Semetal(am)	1.40	-5.79	-7.19	Se
Semetal(hex)	2.03	-5.79	-7.82	Se
SeO ₂	-16.96	-16.85	0.11	SeO ₂
SeO ₃	-59.72	-37.66	22.06	SeO ₃
Siderite	0.60	-9.53	-10.13	FeCO ₃
Thenardite	-8.05	-7.67	0.39	Na ₂ SO ₄
Thermonatrite	-10.73	-10.02	0.71	Na ₂ CO ₃ ·H ₂ O
U ₃ O ₈	-17.82	6.64	24.46	U ₃ O ₈
U ₄ O ₉	-19.26	-19.31	-0.05	U ₄ O ₉
UO ₂ (am)	-10.75	-9.05	1.70	UO ₂
UO ₂ (NO ₃) ₂	-42.42	-29.69	12.73	UO ₂ (NO ₃) ₂
UO ₂ (NO ₃) ₂ ·2H ₂ O	-34.72	-29.69	5.03	UO ₂ (NO ₃) ₂ ·2H ₂ O
UO ₂ (NO ₃) ₂ ·3H ₂ O	-33.14	-29.69	3.45	UO ₂ (NO ₃) ₂ ·3H ₂ O
UO ₂ (NO ₃) ₂ ·6H ₂ O	-31.59	-29.69	1.90	UO ₂ (NO ₃) ₂ ·6H ₂ O
UO ₂ (OH) ₂ (beta)	-8.38	-2.37	6.01	UO ₂ (OH) ₂
UO ₂ SeO ₄ ·4H ₂ O	-37.78	-40.03	-2.25	UO ₂ SeO ₄ ·4H ₂ O
UO ₃	-10.64	-2.37	8.26	UO ₃
Uraninite	-4.92	-9.05	-4.13	UO ₂

**For a gas, SI = log₁₀(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

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

Elements	Molality	Moles
Alkalinity	2.741e-03	2.741e-03
Ca	5.896e-03	5.896e-03
Cl	1.299e-03	1.299e-03
Fe(2)	5.343e-05	5.343e-05
Fe(3)	1.076e-06	1.076e-06
K	1.181e-04	1.181e-04
Mg	2.324e-03	2.324e-03
Mn	1.185e-04	1.185e-04
Mo	1.806e-07	1.806e-07
N(-3)	1.737e-05	1.737e-05
N(5)	1.430e-06	1.430e-06
Na	3.227e-03	3.227e-03
O(0)	1.127e-05	1.127e-05
S(6)	8.016e-03	8.016e-03
Se	1.775e-09	1.775e-09
U	1.275e-08	1.275e-08

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

pH = 7.690
 pe = 0.900
 Activity of water = 1.000
 Ionic strength (mol/kgw) = 2.798e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 2.836e-03
 Total CO2 (mol/kg) = 2.836e-03
 Temperature (°C) = 13.80
 Electrical balance (eq) = 7.436e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.23
 Iterations = 13 (371 overall)
 Total H = 1.110167e+02
 Total O = 5.554742e+01

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

Redox couple	pe	Eh (volts)
Fe(2)/Fe(3)	1.1912	0.0678
N(-3)/N(5)	5.8082	0.3307
O(-2)/O(0)	13.3197	0.7583

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

Species	Molality	Log Activity	Log Molality	Log Activity	mole V	Gamma	cm ³ /mol
OH-	2.407e-07	2.047e-07	-6.618	-6.689	-0.070	(0)	
H+	2.385e-08	2.042e-08	-7.622	-7.690	-0.068	0.00	
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.03	
C(4)	2.836e-03						
HCO3-	2.584e-03	2.227e-03	-2.588	-2.652	-0.065	(0)	
H2CO3	1.181e-04	1.181e-04	-3.928	-3.928	0.000	(0)	
CaHCO3+	8.080e-05	6.988e-05	-4.093	-4.156	-0.063	(0)	
MgHCO3+	2.408e-05	2.056e-05	-4.618	-4.687	-0.069	(0)	
CaCO3	1.156e-05	1.156e-05	-4.937	-4.937	0.000	(0)	
CO3-2	7.569e-06	4.063e-06	-5.121	-5.391	-0.270	(0)	
NaHCO3	4.218e-06	4.218e-06	-5.375	-5.375	0.000	(0)	
MgCO3	2.688e-06	2.688e-06	-5.571	-5.571	0.000	(0)	
MnHCO3+	2.125e-06	1.826e-06	-5.673	-5.738	-0.066	(0)	
FeHCO3+	4.770e-07	4.125e-07	-6.321	-6.385	-0.063	(0)	
NaCO3-	3.282e-07	2.828e-07	-6.484	-6.548	-0.065	(0)	

Ca2UO2(CO3)3	1.017e-08	1.024e-08	-7.993	-7.990	0.003	(0)
CaUO2(CO3)3-2	2.494e-09	1.339e-09	-8.603	-8.873	-0.270	(0)
UO2(CO3)3-4	6.265e-11	2.862e-12	-10.203	-11.543	-1.340	(0)
UO2(CO3)2-2	1.259e-11	5.821e-12	-10.900	-11.235	-0.335	(0)
MgUO2(CO3)3-2	7.179e-12	3.854e-12	-11.144	-11.414	-0.270	(0)
UO2CO3	8.673e-14	8.673e-14	-13.062	-13.062	0.000	(0)
(UO2)2CO3(OH)3-	2.919e-18	2.499e-18	-17.535	-17.602	-0.068	(0)
(UO2)3(CO3)6-6	7.379e-28	2.729e-30	-27.132	-29.564	-2.432	(0)
Ca	5.896e-03					
Ca+2	4.302e-03	2.309e-03	-2.366	-2.637	-0.270	(0)
CaSO4	1.502e-03	1.502e-03	-2.823	-2.823	0.000	(0)
CaHCO3+	8.080e-05	6.988e-05	-4.093	-4.156	-0.063	(0)
CaCO3	1.156e-05	1.156e-05	-4.937	-4.937	0.000	(0)
CaNO3+	1.170e-08	9.649e-09	-7.932	-8.016	-0.084	(0)
Ca2UO2(CO3)3	1.017e-08	1.024e-08	-7.993	-7.990	0.003	(0)
CaOH+	9.571e-09	8.278e-09	-8.019	-8.082	-0.063	(0)
CaUO2(CO3)3-2	2.494e-09	1.339e-09	-8.603	-8.873	-0.270	(0)
CaNH3+2	2.466e-09	1.140e-09	-8.608	-8.943	-0.335	(0)
Ca(NH3)2+2	3.850e-16	1.780e-16	-15.415	-15.750	-0.335	(0)
Cl	1.299e-03					
Cl-	1.299e-03	1.112e-03	-2.886	-2.954	-0.068	(0)
MnCl+	7.131e-08	6.129e-08	-7.147	-7.213	-0.066	(0)
MnCl2	9.627e-11	9.627e-11	-10.017	-10.017	0.000	(0)
MnCl3-	3.431e-14	2.948e-14	-13.465	-13.530	-0.066	(0)
FeCl+2	5.844e-19	3.189e-19	-18.233	-18.496	-0.263	(0)
UO2Cl+	9.709e-21	8.006e-21	-20.013	-20.097	-0.084	(0)
FeCl2+	2.647e-21	2.275e-21	-20.577	-20.643	-0.066	(0)
UO2Cl2	5.258e-25	5.292e-25	-24.279	-24.276	0.003	(0)
FeCl3	2.530e-25	2.530e-25	-24.597	-24.597	0.000	(0)
UCl+3	1.084e-40	0.000e+00	-39.965	-40.719	-0.754	(0)
Fe(2)	5.343e-05					
Fe+2	4.005e-05	1.852e-05	-4.397	-4.732	-0.335	(0)
FeSO4	1.273e-05	1.273e-05	-4.895	-4.895	0.000	(0)
FeHCO3+	4.770e-07	4.125e-07	-6.321	-6.385	-0.063	(0)
FeOH+	1.756e-07	1.509e-07	-6.755	-6.821	-0.066	(0)
Fe(OH)2	2.164e-11	2.164e-11	-10.665	-10.665	0.000	(0)
Fe(OH)3-	3.527e-12	3.031e-12	-11.453	-11.518	-0.066	(0)
Fe(3)	1.076e-06					
Fe(OH)2+	9.663e-07	8.326e-07	-6.015	-6.080	-0.065	(0)
Fe(OH)3	8.600e-08	8.600e-08	-7.065	-7.065	0.000	(0)
Fe(OH)4-	2.349e-08	2.024e-08	-7.629	-7.694	-0.065	(0)
FeOH+2	4.120e-12	2.248e-12	-11.385	-11.648	-0.263	(0)
FeSO4+	3.815e-16	3.278e-16	-15.419	-15.484	-0.066	(0)
Fe+3	5.530e-17	1.364e-17	-16.257	-16.865	-0.608	(0)
Fe(SO4)2-	2.958e-17	2.439e-17	-16.529	-16.613	-0.084	(0)
FeCl+2	5.844e-19	3.189e-19	-18.233	-18.496	-0.263	(0)
Fe2(OH)2+4	5.513e-21	2.519e-22	-20.259	-21.599	-1.340	(0)
FeCl2+	2.647e-21	2.275e-21	-20.577	-20.643	-0.066	(0)
FeNO3+2	6.411e-22	2.964e-22	-21.193	-21.528	-0.335	(0)
FeHSeO3+2	5.826e-23	2.694e-23	-22.235	-22.570	-0.335	(0)
Fe3(OH)4+5	3.338e-25	2.689e-27	-24.476	-26.570	-2.094	(0)
FeCl3	2.530e-25	2.530e-25	-24.597	-24.597	0.000	(0)
H(0)	1.044e-20					
H2	5.218e-21	5.252e-21	-20.282	-20.280	0.003	(0)
K	1.181e-04					
K+	1.156e-04	9.898e-05	-3.937	-4.004	-0.068	(0)
KSO4-	2.421e-06	2.086e-06	-5.616	-5.681	-0.065	(0)
Mg	2.324e-03					
Mg+2	1.790e-03	9.608e-04	-2.747	-3.017	-0.270	(0)
MgSO4	5.068e-04	5.068e-04	-3.295	-3.295	0.000	(0)
MgHCO3+	2.408e-05	2.056e-05	-4.618	-4.687	-0.069	(0)
MgCO3	2.688e-06	2.688e-06	-5.571	-5.571	0.000	(0)
MgOH+	7.475e-08	6.483e-08	-7.126	-7.188	-0.062	(0)
MgUO2(CO3)3-2	7.179e-12	3.854e-12	-11.144	-11.414	-0.270	(0)
Mn(2)	1.185e-04					
Mn+2	9.469e-05	4.378e-05	-4.024	-4.359	-0.335	(0)

MnSO4	2.156e-05	2.156e-05	-4.666	-4.666	0.000	(0)
MnHCO3+	2.125e-06	1.826e-06	-5.673	-5.738	-0.066	(0)
MnCl+	7.131e-08	6.129e-08	-7.147	-7.213	-0.066	(0)
MnOH+	2.620e-08	2.252e-08	-7.582	-7.648	-0.066	(0)
MnNO3+	1.021e-10	8.421e-11	-9.991	-10.075	-0.084	(0)
MnCl2	9.627e-11	9.627e-11	-10.017	-10.017	0.000	(0)
MnCl3-	3.431e-14	2.948e-14	-13.465	-13.530	-0.066	(0)
Mn(NO3)2	2.635e-16	2.635e-16	-15.579	-15.579	0.000	(0)
Mn(OH)3-	9.475e-17	8.143e-17	-16.023	-16.089	-0.066	(0)
MnSe	2.048e-18	2.048e-18	-17.689	-17.689	0.000	(0)
Mn(OH)4-2	2.376e-22	1.296e-22	-21.624	-21.887	-0.263	(0)
MnSeO4	1.607e-24	1.607e-24	-23.794	-23.794	0.000	(0)
Mn(3)	1.154e-29					
Mn+3	1.154e-29	2.845e-30	-28.938	-29.546	-0.608	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-62.260	-62.524	-0.263	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-71.687	-71.759	-0.072	(0)
Mo	1.806e-07					
MoO4-2	1.805e-07	9.690e-08	-6.743	-7.014	-0.270	(0)
HMoO4-	3.484e-11	2.873e-11	-10.458	-10.542	-0.084	(0)
H2MoO4	8.866e-15	8.866e-15	-14.052	-14.052	0.000	(0)
Mo7O24-6	0.000e+00	0.000e+00	-53.051	-56.066	-3.015	(0)
HMo7O24-5	0.000e+00	0.000e+00	-55.344	-57.438	-2.094	(0)
H2Mo7O24-4	0.000e+00	0.000e+00	-59.026	-60.366	-1.340	(0)
H3Mo7O24-3	0.000e+00	0.000e+00	-64.042	-64.796	-0.754	(0)
N(-3)	1.737e-05					
NH4+	1.664e-05	1.404e-05	-4.779	-4.853	-0.074	(0)
NH4SO4-	5.560e-07	4.779e-07	-6.255	-6.321	-0.066	(0)
NH3	1.729e-07	1.729e-07	-6.762	-6.762	0.000	(0)
CaNH3+2	2.466e-09	1.140e-09	-8.608	-8.943	-0.335	(0)
Ca(NH3)2+2	3.850e-16	1.780e-16	-15.415	-15.750	-0.335	(0)
N(5)	1.430e-06					
NO3-	1.418e-06	1.214e-06	-5.848	-5.916	-0.068	(0)
CaNO3+	1.170e-08	9.649e-09	-7.932	-8.016	-0.084	(0)
MnNO3+	1.021e-10	8.421e-11	-9.991	-10.075	-0.084	(0)
Mn(NO3)2	2.635e-16	2.635e-16	-15.579	-15.579	0.000	(0)
FeNO3+2	6.411e-22	2.964e-22	-21.193	-21.528	-0.335	(0)
UO2NO3+	2.026e-23	1.671e-23	-22.693	-22.777	-0.084	(0)
Na	3.227e-03					
Na+	3.170e-03	2.713e-03	-2.499	-2.566	-0.068	(0)
NaSO4-	5.287e-05	4.555e-05	-4.277	-4.341	-0.065	(0)
NaHCO3	4.218e-06	4.218e-06	-5.375	-5.375	0.000	(0)
NaCO3-	3.282e-07	2.828e-07	-6.484	-6.548	-0.065	(0)
O(0)	1.127e-05					
O2	5.633e-06	5.669e-06	-5.249	-5.247	0.003	(0)
S(6)	8.016e-03					
SO4-2	5.916e-03	3.176e-03	-2.228	-2.498	-0.270	(0)
CaSO4	1.502e-03	1.502e-03	-2.823	-2.823	0.000	(0)
MgSO4	5.068e-04	5.068e-04	-3.295	-3.295	0.000	(0)
NaSO4-	5.287e-05	4.555e-05	-4.277	-4.341	-0.065	(0)
MnSO4	2.156e-05	2.156e-05	-4.666	-4.666	0.000	(0)
FeSO4	1.273e-05	1.273e-05	-4.895	-4.895	0.000	(0)
KSO4-	2.421e-06	2.086e-06	-5.616	-5.681	-0.065	(0)
NH4SO4-	5.560e-07	4.779e-07	-6.255	-6.321	-0.066	(0)
HSO4-	5.232e-09	4.481e-09	-8.281	-8.349	-0.067	(0)
FeSO4+	3.815e-16	3.278e-16	-15.419	-15.484	-0.066	(0)
Fe(SO4)2-	2.958e-17	2.439e-17	-16.529	-16.613	-0.084	(0)
UO2SO4	2.004e-17	2.004e-17	-16.698	-16.698	0.000	(0)
UO2(SO4)2-2	1.366e-18	6.318e-19	-17.864	-18.199	-0.335	(0)
U(SO4)2	4.747e-35	4.747e-35	-34.324	-34.324	0.000	(0)
USO4+2	6.033e-36	2.789e-36	-35.219	-35.555	-0.335	(0)
Se(-2)	2.831e-16					
HSe-	2.810e-16	2.317e-16	-15.551	-15.635	-0.084	(0)
MnSe	2.048e-18	2.048e-18	-17.689	-17.689	0.000	(0)
H2Se	3.487e-20	3.487e-20	-19.458	-19.458	0.000	(0)

Se-2 1.151e-23 5.321e-24 -22.939 -23.274 -0.335 (0)
 Se(4) 1.775e-09
 HSeO3- 1.344e-09 1.108e-09 -8.872 -8.955 -0.084 (0)
 SeO3-2 4.318e-10 1.996e-10 -9.365 -9.700 -0.335 (0)
 H2SeO3 8.752e-15 8.752e-15 -14.058 -14.058 0.000 (0)
 FeHSeO3+2 5.826e-23 2.694e-23 -22.235 -22.570 -0.335 (0)
 Se(6) 3.184e-22
 SeO4-2 3.168e-22 1.701e-22 -21.499 -21.769 -0.270 (0)
 MnSeO4 1.607e-24 1.607e-24 -23.794 -23.794 0.000 (0)
 HSeO4- 1.469e-28 1.212e-28 -27.833 -27.917 -0.084 (0)
 U(3) 0.000e+00
 U+3 0.000e+00 0.000e+00 -49.242 -49.996 -0.754 (0)
 U(4) 1.054e-15
 U(OH)5- 1.053e-15 8.682e-16 -14.978 -15.061 -0.084 (0)
 U(OH)4 8.940e-19 8.940e-19 -18.049 -18.049 0.000 (0)
 U(OH)3+ 9.306e-23 7.674e-23 -22.031 -22.115 -0.084 (0)
 U(OH)2+2 2.167e-27 1.002e-27 -26.664 -26.999 -0.335 (0)
 UOH+3 8.282e-33 1.460e-33 -32.082 -32.836 -0.754 (0)
 U(SO4)2 4.747e-35 4.747e-35 -34.324 -34.324 0.000 (0)
 USO4+2 6.033e-36 2.789e-36 -35.219 -35.555 -0.335 (0)
 U+4 5.477e-39 2.502e-40 -38.261 -39.602 -1.340 (0)
 UCl+3 1.084e-40 0.000e+00 -39.965 -40.719 -0.754 (0)
 U6(OH)15+9 0.000e+00 0.000e+00 -132.633 -139.417 -6.785 (0)
 U(5) 6.604e-16
 UO2+ 6.604e-16 5.446e-16 -15.180 -15.264 -0.084 (0)
 U(6) 1.275e-08
 Ca2UO2(CO3)3 1.017e-08 1.024e-08 -7.993 -7.990 0.003 (0)
 CaUO2(CO3)3-2 2.494e-09 1.339e-09 -8.603 -8.873 -0.270 (0)
 UO2(CO3)3-4 6.265e-11 2.862e-12 -10.203 -11.543 -1.340 (0)
 UO2(CO3)2-2 1.259e-11 5.821e-12 -10.900 -11.235 -0.335 (0)
 MgUO2(CO3)3-2 7.179e-12 3.854e-12 -11.144 -11.414 -0.270 (0)
 UO2(OH)2 6.591e-13 6.634e-13 -12.181 -12.178 0.003 (0)
 UO2CO3 8.673e-14 8.673e-14 -13.062 -13.062 0.000 (0)
 UO2(OH)3- 4.699e-14 4.022e-14 -13.328 -13.396 -0.068 (0)
 UO2OH+ 2.025e-16 1.670e-16 -15.694 -15.777 -0.084 (0)
 UO2SO4 2.004e-17 2.004e-17 -16.698 -16.698 0.000 (0)
 UO2+2 1.064e-17 5.711e-18 -16.973 -17.243 -0.270 (0)
 (UO2)2CO3(OH)3- 2.919e-18 2.499e-18 -17.535 -17.602 -0.068 (0)
 UO2(SO4)2-2 1.366e-18 6.318e-19 -17.864 -18.199 -0.335 (0)
 UO2(OH)4-2 5.717e-20 3.069e-20 -19.243 -19.513 -0.270 (0)
 UO2Cl+ 9.709e-21 8.006e-21 -20.013 -20.097 -0.084 (0)
 UO2NO3+ 2.026e-23 1.671e-23 -22.693 -22.777 -0.084 (0)
 UO2Cl2 5.258e-25 5.292e-25 -24.279 -24.276 0.003 (0)
 (UO2)2(OH)2+2 2.334e-25 1.079e-25 -24.632 -24.967 -0.335 (0)
 (UO2)3(CO3)6-6 7.379e-28 2.729e-30 -27.132 -29.564 -2.432 (0)
 (UO2)3(OH)7- 1.305e-29 1.117e-29 -28.884 -28.952 -0.068 (0)
 (UO2)2OH+3 1.271e-29 3.134e-30 -28.896 -29.504 -0.608 (0)
 (UO2)3(OH)5+ 3.015e-30 2.486e-30 -29.521 -29.605 -0.084 (0)
 (UO2)3(OH)4+2 2.348e-33 1.260e-33 -32.629 -32.900 -0.270 (0)
 (UO2)4(OH)7+ 9.385e-38 8.033e-38 -37.028 -37.095 -0.068 (0)

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

Phase SI** log IAP log K(286 K, 1 atm)

(NH4)2SeO4 -31.92 -31.47 0.45 (NH4)2SeO4
 Anhydrite -0.82 -5.13 -4.31 CaSO4
 Aragonite 0.19 -8.03 -8.22 CaCO3
 Artinite -6.47 3.95 10.42 MgCO3:Mg(OH)2:3H2O
 Birnessite -15.98 2.11 18.09 MnO2
 Bixbyite -13.16 -12.95 0.21 Mn2O3
 Brucite -5.26 12.36 17.62 Mg(OH)2
 Calcite 0.40 -8.03 -8.43 CaCO3
 CaMoO4 -1.71 -9.65 -7.94 CaMoO4
 CaSeO3:2H2O -6.85 -3.90 2.95 CaSeO3:2H2O
 CaSeO4:2H2O -21.44 -24.41 -2.96 CaSeO4:2H2O

CH4(g)	-46.69	-89.49	-42.80	CH4
CO2(g)	-2.60	-20.77	-18.17	CO2
Dolomite(disordered)	-0.21	-16.44	-16.22	CaMg(CO3)2
Dolomite(ordered)	0.38	-16.44	-16.82	CaMg(CO3)2
Epsomite	-3.31	-5.52	-2.21	MgSO4:7H2O
Fe(OH)2	-2.92	10.65	13.56	Fe(OH)2
Fe(OH)2.7Cl.3	6.05	3.01	-3.04	Fe(OH)2.7Cl.3
Fe2(OH)4SeO3	-5.79	-4.24	1.55	Fe2(OH)4SeO3
Fe2(SeO3)3:2H2O	-16.90	-37.53	-20.63	Fe2(SeO3)3:2H2O
Fe2(SO4)3	-39.15	-41.22	-2.08	Fe2(SO4)3
Fe3(OH)8	2.83	23.06	20.22	Fe3(OH)8
FeMoO4	-1.73	-11.75	-10.02	FeMoO4
Ferrihydrite	2.51	6.20	3.69	Fe(OH)3
Ferroselite	0.10	-18.82	-18.92	FeSe2
FeSe	-1.66	-12.68	-11.01	FeSe
Goethite	5.30	6.20	0.91	FeOOH
Gummitite	-10.09	-1.86	8.23	UO3
Gypsum	-0.52	-5.14	-4.62	CaSO4:2H2O
H-Jarosite	-6.62	-17.14	-10.52	(H3O)Fe3(SO4)2(OH)6
H2MoO4	-9.18	-22.39	-13.21	H2MoO4
H2Se(g)	-18.47	-23.32	-4.86	H2Se
Halite	-7.10	-5.52	1.58	NaCl
Hausmannite	-13.67	50.24	63.91	Mn3O4
Hematite	12.95	12.41	-0.54	Fe2O3
Huntite	-4.02	-33.25	-29.23	CaMg3(CO3)4
Hydromagnesite	-14.00	-21.27	-7.27	Mg5(CO3)4(OH)2:4H2O
K-Jarosite	0.45	-13.46	-13.91	KFe3(SO4)2(OH)6
K2MoO4	-18.31	-15.02	3.29	K2MoO4
K2SeO4	-29.05	-29.78	-0.73	K2SeO4
Lepidocrocite	4.83	6.20	1.37	FeOOH
Lime	-21.28	12.74	34.03	CaO
Maghemite	6.02	12.41	6.39	Fe2O3
Magnesianoferrite	6.00	24.77	18.77	Fe2MgO4
Magnetite	-0.81	-8.41	-7.60	MgCO3
Magnetite	18.23	23.06	4.83	Fe3O4
Manganite	-5.73	19.61	25.34	MnOOH
Melanterite	-4.88	-7.23	-2.35	FeSO4:7H2O
Mg(OH)2(active)	-6.43	12.36	18.79	Mg(OH)2
MgMoO4	-8.18	-10.03	-1.85	MgMoO4
MgSeO3:6H2O	-7.30	-4.28	3.02	MgSeO3:6H2O
MgSeO4:6H2O	-23.59	-24.79	-1.20	MgSeO4:6H2O
Mirabilite	-5.98	-7.63	-1.66	Na2SO4:10H2O
Mn2(SO4)3	-61.99	-66.59	-4.59	Mn2(SO4)3
MnCl2:4H2O	-13.06	-10.27	2.79	MnCl2:4H2O
MnSe	-16.47	-12.30	4.17	MnSe
MnSeO3	-6.75	-5.62	1.13	MnSeO3
MnSeO3:2H2O	-6.55	-5.62	0.92	MnSeO3:2H2O
MnSeO4:5H2O	-24.08	-26.13	-2.05	MnSeO4:5H2O
MnSO4	-9.88	-6.86	3.03	MnSO4
MoO3	-14.39	-22.39	-8.00	MoO3
Na-Jarosite	-1.85	-12.02	-10.16	NaFe3(SO4)2(OH)6
Na2Mo2O7	-17.56	-34.54	-16.98	Na2Mo2O7
Na2MoO4	-13.70	-12.15	1.56	Na2MoO4
Na2MoO4:2H2O	-13.37	-12.15	1.22	Na2MoO4:2H2O
Na2SeO3:5H2O	-16.70	-6.40	10.30	Na2SeO3:5H2O
Na2SeO4	-28.18	-26.90	1.28	Na2SeO4
Natron	-8.76	-10.53	-1.76	Na2CO3:10H2O
Nesquehonite	-3.90	-8.41	-4.50	MgCO3:3H2O
Nsutite	-15.39	2.11	17.50	MnO2
O2(g)	-52.64	34.36	87.00	O2
Periclase	-10.26	12.36	22.62	MgO
Portlandite	-10.94	12.74	23.68	Ca(OH)2
Pyrochroite	-4.84	11.02	15.86	Mn(OH)2
Pyrolusite	-15.04	28.20	43.24	MnO2
Rhodochrosite	0.82	-9.75	-10.57	MnCO3
Rutherfordine	-8.16	-22.63	-14.48	UO2CO3

Schoepite	-8.20	-1.86	6.33	UO ₂ (OH) ₂ :H ₂ O
Semetal(am)	1.04	-6.14	-7.18	Se
Semetal(hex)	1.67	-6.14	-7.82	Se
SeO ₂	-16.76	-16.65	0.12	SeO ₂
SeO ₃	-59.19	-37.15	22.04	SeO ₃
Siderite	0.01	-10.12	-10.13	FeCO ₃
Thenardite	-8.02	-7.63	0.38	Na ₂ SO ₄
Thermonatrite	-11.23	-10.52	0.71	Na ₂ CO ₃ :H ₂ O
U ₃ O ₈	-16.57	7.83	24.40	U ₃ O ₈
U ₄ O ₉	-18.09	-18.19	-0.10	U ₄ O ₉
UO ₂ (am)	-10.53	-8.84	1.68	UO ₂
UO ₂ (NO ₃) ₂	-41.79	-29.08	12.72	UO ₂ (NO ₃) ₂
UO ₂ (NO ₃) ₂ :2H ₂ O	-34.10	-29.08	5.02	UO ₂ (NO ₃) ₂ :2H ₂ O
UO ₂ (NO ₃) ₂ :3H ₂ O	-32.53	-29.08	3.45	UO ₂ (NO ₃) ₂ :3H ₂ O
UO ₂ (NO ₃) ₂ :6H ₂ O	-30.98	-29.08	1.90	UO ₂ (NO ₃) ₂ :6H ₂ O
UO ₂ (OH) ₂ (beta)	-7.86	-1.86	6.00	UO ₂ (OH) ₂
UO ₂ SeO ₄ :4H ₂ O	-36.76	-39.01	-2.25	UO ₂ SeO ₄ :4H ₂ O
UO ₃	-10.12	-1.86	8.25	UO ₃
Uraninite	-4.71	-8.84	-4.14	UO ₂

**For a gas, SI = log₁₀(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.307 Seconds.
