

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

LLNL\_AQUEOUS\_MODEL\_PARAMETERS  
NAMED\_EXPRESSIONS  
SOLUTION\_MASTER\_SPECIES  
SOLUTION\_SPECIES  
PHASES  
EXCHANGE\_MASTER\_SPECIES  
EXCHANGE\_SPECIES  
SURFACE\_MASTER\_SPECIES  
SURFACE\_SPECIES  
RATES  
END

-----  
Reading input data for simulation 1.  
-----

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat  
SOLUTION 1 Flujo 4  
temp 25  
pH 3.17  
pe 12  
redox pe  
units mg/l  
density 1  
Cl 46.9  
S(6) 1089.6  
Al 25.6  
As 5.0  
Ca 201.4  
Cu 35.1  
Fe 170.2  
K 69.2  
Mg 19.8  
Mn 20.6  
Na 33.2  
Zn 17.4  
C(4) 0  
water 1 # kg  
SOLUTION 4 AS3  
temp 25  
units mg/l  
pe 10  
pH 7.74  
Cl 24.2  
S(6) 243.00  
Al 0.00  
As 0.0966  
Ca 86.82  
Cu 0.113  
Fe 0.00  
K 3.07  
Mg 16.17  
Mn 0.181  
Na 43.01  
Zn 0.195  
C(4) 115.9  
MIX 4  
1 1

```

4      1
SELECTED_OUTPUT
file          DAM_AGUASUP
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

```

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

Initial solution 1.      Flujo 4

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

Elements	Molality	Moles
Al	9.504e-004	9.504e-004
As	6.685e-005	6.685e-005
Ca	5.034e-003	5.034e-003
Cl	1.325e-003	1.325e-003
Cu	5.533e-004	5.533e-004
Fe	3.053e-003	3.053e-003
K	1.773e-003	1.773e-003
Mg	8.161e-004	8.161e-004
Mn	3.756e-004	3.756e-004
Na	1.447e-003	1.447e-003
S(6)	1.136e-002	1.136e-002
Zn	2.666e-004	2.666e-004

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

```

pH = 3.170
pe = 12.000
Activity of water = 1.000
Ionic strength = 3.718e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -2.718e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = 3.154e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 8.05
Iterations = 8
Total H = 1.110537e+002
Total O = 5.557286e+001

```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	7.785e-004	6.761e-004	-3.109	-3.170	-0.061
OH-	1.709e-011	1.424e-011	-10.767	-10.846	-0.079
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	9.504e-004				
AlSO4+	4.577e-004	3.832e-004	-3.339	-3.417	-0.077
Al+3	3.507e-004	9.580e-005	-3.455	-4.019	-0.564
Al(SO4)2-	1.389e-004	1.163e-004	-3.857	-3.935	-0.077
AlOH+2	3.206e-006	1.587e-006	-5.494	-5.799	-0.305
Al(OH)2+	6.507e-009	5.448e-009	-8.187	-8.264	-0.077
Al2(OH)2+4	6.033e-009	4.095e-010	-8.219	-9.388	-1.168
HALO2	1.173e-011	1.173e-011	-10.931	-10.931	0.000
Al3(OH)4+5	3.369e-012	5.535e-014	-11.472	-13.257	-1.784
AlO2-	7.097e-015	5.942e-015	-14.149	-14.226	-0.077
NaAlO2	1.338e-018	1.338e-018	-17.874	-17.874	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-46.038	-49.537	-3.499

As(-3)	0.000e+000					
AsH3	0.000e+000	0.000e+000	-112.033	-112.033	0.000	
As(3)	1.610e-016					
HAsO2	8.593e-017	8.593e-017	-16.066	-16.066	0.000	
As(OH)3	7.510e-017	7.510e-017	-16.124	-16.124	0.000	
H2AsO3-	8.114e-023	6.793e-023	-22.091	-22.168	-0.077	
AsO2-	7.760e-023	6.497e-023	-22.110	-22.187	-0.077	
AsO2OH-2	2.019e-030	9.817e-031	-29.695	-30.008	-0.313	
As(5)	6.685e-005					
H2AsO4-	6.077e-005	5.088e-005	-4.216	-4.293	-0.077	
H3AsO4	6.059e-006	6.059e-006	-5.218	-5.218	0.000	
HAsO4-2	2.569e-008	1.249e-008	-7.590	-7.903	-0.313	
AsO4-3	2.411e-016	4.740e-017	-15.618	-16.324	-0.706	
Ca	5.034e-003					
Ca+2	3.882e-003	2.017e-003	-2.411	-2.695	-0.284	
CaSO4	1.152e-003	1.152e-003	-2.939	-2.939	0.000	
CaCl+	5.599e-007	4.688e-007	-6.252	-6.329	-0.077	
CaCl2	6.044e-010	6.044e-010	-9.219	-9.219	0.000	
CaOH+	5.032e-013	4.213e-013	-12.298	-12.375	-0.077	
Cl(-1)	1.325e-003					
Cl-	1.322e-003	1.096e-003	-2.879	-2.960	-0.081	
CuCl+	7.019e-007	5.877e-007	-6.154	-6.231	-0.077	
CaCl+	5.599e-007	4.688e-007	-6.252	-6.329	-0.077	
FeCl+	5.035e-007	4.215e-007	-6.298	-6.375	-0.077	
MnCl+	3.622e-007	3.033e-007	-6.441	-6.518	-0.077	
MgCl+	2.911e-007	2.438e-007	-6.536	-6.613	-0.077	
NaCl	2.275e-007	2.275e-007	-6.643	-6.643	0.000	
ZnCl+	2.134e-007	1.787e-007	-6.671	-6.748	-0.077	
HCl	1.665e-007	1.665e-007	-6.779	-6.779	0.000	
KCl	5.248e-008	5.248e-008	-7.280	-7.280	0.000	
FeCl+2	1.867e-008	9.244e-009	-7.729	-8.034	-0.305	
FeCl2+	9.799e-009	8.204e-009	-8.009	-8.086	-0.077	
CaCl2	6.044e-010	6.044e-010	-9.219	-9.219	0.000	
CuCl2	3.393e-010	3.393e-010	-9.469	-9.469	0.000	
ZnCl2	2.288e-010	2.288e-010	-9.640	-9.640	0.000	
Zn(OH)Cl	4.517e-012	4.517e-012	-11.345	-11.345	0.000	
FeCl2	2.480e-012	2.480e-012	-11.606	-11.606	0.000	
ZnCl3-	1.655e-013	1.385e-013	-12.781	-12.858	-0.077	
MnCl3-	9.510e-014	7.962e-014	-13.022	-13.099	-0.077	
CuCl2-	1.020e-014	8.543e-015	-13.991	-14.068	-0.077	
ZnCl4-2	2.368e-015	1.151e-015	-14.626	-14.939	-0.313	
CuCl3-2	1.237e-016	6.015e-017	-15.908	-16.221	-0.313	
FeCl4-2	1.771e-017	8.612e-018	-16.752	-17.065	-0.313	
FeCl4-	1.416e-017	1.185e-017	-16.849	-16.926	-0.077	
CuCl4-2	1.574e-020	7.653e-021	-19.803	-20.116	-0.313	
Cl(1)	4.682e-027					
HClO	4.682e-027	4.682e-027	-26.330	-26.330	0.000	
ClO-	2.230e-031	1.867e-031	-30.652	-30.729	-0.077	
Cl(3)	0.000e+000					
ClO2-	0.000e+000	0.000e+000	-51.315	-51.392	-0.077	
HClO2	0.000e+000	0.000e+000	-51.392	-51.392	0.000	
Cl(5)	0.000e+000					
ClO3-	0.000e+000	0.000e+000	-58.124	-58.203	-0.079	
Cl(7)	0.000e+000					
ClO4-	0.000e+000	0.000e+000	-69.237	-69.316	-0.079	
ZnClO4+	0.000e+000	0.000e+000	-71.975	-72.052	-0.077	
Cu(1)	1.385e-013					
Cu+	1.281e-013	1.073e-013	-12.892	-12.969	-0.077	
CuCl2-	1.020e-014	8.543e-015	-13.991	-14.068	-0.077	
CuCl3-2	1.237e-016	6.015e-017	-15.908	-16.221	-0.313	
Cu(2)	5.533e-004					
Cu+2	3.771e-004	1.960e-004	-3.424	-3.708	-0.284	
CuSO4	1.755e-004	1.755e-004	-3.756	-3.756	0.000	
CuCl+	7.019e-007	5.877e-007	-6.154	-6.231	-0.077	
CuOH+	1.785e-008	1.495e-008	-7.748	-7.825	-0.077	
CuCl2	3.393e-010	3.393e-010	-9.469	-9.469	0.000	
CuCl4-2	1.574e-020	7.653e-021	-19.803	-20.116	-0.313	

CuO2-2	6.844e-031	3.328e-031	-30.165	-30.478	-0.313
Fe(2)	1.343e-003				
Fe+2	1.016e-003	5.278e-004	-2.993	-3.278	-0.284
FeSO4	3.270e-004	3.270e-004	-3.486	-3.486	0.000
FeCl+	5.035e-007	4.215e-007	-6.298	-6.375	-0.077
FeOH+	2.947e-010	2.468e-010	-9.531	-9.608	-0.077
FeCl2	2.480e-012	2.480e-012	-11.606	-11.606	0.000
FeCl4-2	1.771e-017	8.612e-018	-16.752	-17.065	-0.313
Fe(OH)2	2.898e-018	2.898e-018	-17.538	-17.538	0.000
Fe(OH)3-	2.037e-025	1.706e-025	-24.691	-24.768	-0.077
Fe(OH)4-2	5.187e-037	2.522e-037	-36.285	-36.598	-0.313
Fe(3)	1.710e-003				
FeOH+2	9.759e-004	4.831e-004	-3.011	-3.316	-0.305
Fe(OH)2+	2.825e-004	2.365e-004	-3.549	-3.626	-0.077
Fe+3	1.852e-004	5.061e-005	-3.732	-4.296	-0.564
Fe2(OH)2+4	9.255e-005	6.281e-006	-4.034	-5.202	-1.168
FeSO4+	2.286e-005	1.914e-005	-4.641	-4.718	-0.077
Fe3(OH)4+5	1.889e-005	3.104e-007	-4.724	-6.508	-1.784
Fe(SO4)2-	1.510e-006	1.265e-006	-5.821	-5.898	-0.077
Fe(OH)3	1.635e-007	1.635e-007	-6.786	-6.786	0.000
FeCl+2	1.867e-008	9.244e-009	-7.729	-8.034	-0.305
FeCl2+	9.799e-009	8.204e-009	-8.009	-8.086	-0.077
Fe(OH)4-	7.254e-014	6.074e-014	-13.139	-13.217	-0.077
FeCl4-	1.416e-017	1.185e-017	-16.849	-16.926	-0.077
H(0)	7.189e-034				
H2	3.595e-034	3.627e-034	-33.444	-33.440	0.004
K	1.773e-003				
K+	1.719e-003	1.426e-003	-2.765	-2.846	-0.081
KSO4-	5.372e-005	4.497e-005	-4.270	-4.347	-0.077
KCl	5.248e-008	5.248e-008	-7.280	-7.280	0.000
KHSO4	2.683e-008	2.683e-008	-7.571	-7.571	0.000
KOH	7.308e-015	7.308e-015	-14.136	-14.136	0.000
Mg	8.161e-004				
Mg+2	5.185e-004	2.848e-004	-3.285	-3.545	-0.260
MgSO4	2.973e-004	2.973e-004	-3.527	-3.527	0.000
MgCl+	2.911e-007	2.438e-007	-6.536	-6.613	-0.077
Mg4(OH)4+4	0.000e+000	0.000e+000	-40.084	-41.252	-1.168
Mn(2)	3.756e-004				
Mn+2	2.500e-004	1.299e-004	-3.602	-3.886	-0.284
MnSO4	1.253e-004	1.253e-004	-3.902	-3.902	0.000
MnCl+	3.622e-007	3.033e-007	-6.441	-6.518	-0.077
MnOH+	5.897e-012	4.937e-012	-11.229	-11.307	-0.077
MnCl3-	9.510e-014	7.962e-014	-13.022	-13.099	-0.077
Mn2OH+3	3.232e-015	6.873e-016	-14.490	-15.163	-0.672
Mn(OH)2	1.792e-020	1.792e-020	-19.747	-19.747	0.000
Mn2(OH)3+	8.202e-023	6.867e-023	-22.086	-22.163	-0.077
Mn(OH)3-	2.968e-029	2.485e-029	-28.528	-28.605	-0.077
Mn(OH)4-2	6.398e-040	3.111e-040	-39.194	-39.507	-0.313
Mn(3)	1.630e-017				
Mn+3	1.630e-017	3.465e-018	-16.788	-17.460	-0.672
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-48.661	-48.974	-0.313
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-46.251	-46.330	-0.079
Na	1.447e-003				
Na+	1.410e-003	1.181e-003	-2.851	-2.928	-0.077
NaSO4-	3.641e-005	3.049e-005	-4.439	-4.516	-0.077
NaCl	2.275e-007	2.275e-007	-6.643	-6.643	0.000
NaOH	2.901e-015	2.901e-015	-14.537	-14.537	0.000
NaAlO2	1.338e-018	1.338e-018	-17.874	-17.874	0.000
O(0)	9.587e-026				
O2	4.793e-026	4.837e-026	-25.319	-25.315	0.004
S(6)	1.136e-002				
SO4-2	8.038e-003	3.909e-003	-2.095	-2.408	-0.313
CaSO4	1.152e-003	1.152e-003	-2.939	-2.939	0.000
AlSO4+	4.577e-004	3.832e-004	-3.339	-3.417	-0.077
FeSO4	3.270e-004	3.270e-004	-3.486	-3.486	0.000

HSO4-	3.188e-004	2.669e-004	-3.496	-3.574	-0.077
MgSO4	2.973e-004	2.973e-004	-3.527	-3.527	0.000
CuSO4	1.755e-004	1.755e-004	-3.756	-3.756	0.000
Al(SO4)2-	1.389e-004	1.163e-004	-3.857	-3.935	-0.077
MnSO4	1.253e-004	1.253e-004	-3.902	-3.902	0.000
ZnSO4	7.968e-005	7.968e-005	-4.099	-4.099	0.000
KSO4-	5.372e-005	4.497e-005	-4.270	-4.347	-0.077
NaSO4-	3.641e-005	3.049e-005	-4.439	-4.516	-0.077
FeSO4+	2.286e-005	1.914e-005	-4.641	-4.718	-0.077
Fe(SO4)2-	1.510e-006	1.265e-006	-5.821	-5.898	-0.077
KHSO4	2.683e-008	2.683e-008	-7.571	-7.571	0.000
H2SO4	1.703e-010	1.703e-010	-9.769	-9.769	0.000
Zn	2.666e-004				
Zn+2	1.867e-004	9.702e-005	-3.729	-4.013	-0.284
ZnSO4	7.968e-005	7.968e-005	-4.099	-4.099	0.000
ZnCl+	2.134e-007	1.787e-007	-6.671	-6.748	-0.077
ZnCl2	2.288e-010	2.288e-010	-9.640	-9.640	0.000
ZnOH+	1.879e-010	1.573e-010	-9.726	-9.803	-0.077
Zn(OH)Cl	4.517e-012	4.517e-012	-11.345	-11.345	0.000
ZnCl3-	1.655e-013	1.385e-013	-12.781	-12.858	-0.077
ZnCl4-2	2.368e-015	1.151e-015	-14.626	-14.939	-0.313
Zn(OH)2	9.960e-016	9.960e-016	-15.002	-15.002	0.000
Zn(OH)3-	5.452e-024	4.565e-024	-23.263	-23.341	-0.077
Zn(OH)4-2	2.366e-033	1.151e-033	-32.626	-32.939	-0.313
ZnClO4+	0.000e+000	0.000e+000	-71.975	-72.052	-0.077

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

Phase	SI	log IAP	log KT	
Al	-125.44	24.48	149.91	Al
Al(g)	-176.14	24.48	200.62	Al
Al2(SO4)3	-34.16	-15.26	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.82	-15.26	1.56	Al2(SO4)3:6H2O
Alum-K	-6.71	-11.68	-4.97	KAl(SO4)2:12H2O
Alunite	-0.23	-0.70	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.75	-5.10	-4.35	CaSO4
Antarcticite	-12.71	-8.62	4.09	CaCl2:6H2O
Antlerite	-9.58	-0.85	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.39	-16.28	-3.89	NaK3(SO4)2
Arcanite	-6.26	-8.10	-1.84	K2SO4
Arsenolite	-30.83	-50.68	-19.84	As2O3
As	-49.03	-6.35	42.68	As
As2O5	-17.06	-14.93	2.14	As2O5
As4O6(cubi)	-61.53	-101.35	-39.82	As4O6
As4O6(mono)	-61.30	-101.35	-40.05	As4O6
Atacamite	-16.00	-1.73	14.26	Cu4Cl2(OH)6
Bassanite	-1.40	-5.10	-3.71	CaSO4:0.5H2O
Birnessite	-68.13	-153.67	-85.55	Mn8O14:5H2O
Bischofite	-13.86	-9.47	4.39	MgCl2:6H2O
Bixbyite	-14.94	-15.90	-0.96	Mn2O3
Bloedite	-11.74	-14.22	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.06	5.49	7.55	AlO2H
Brochantite	-13.64	1.78	15.42	Cu4(SO4)(OH)6
Brucite	-13.49	2.79	16.28	Mg(OH)2
Ca	-123.53	16.30	139.83	Ca
Ca(g)	-148.77	16.30	165.07	Ca
Ca2Al2O5:8H2O	-41.30	18.27	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-31.26	-4.97	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-21.80	-3.99	17.80	Ca3(AsO4)2
Ca3Al2O6	-91.12	21.92	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-104.49	35.99	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-81.70	25.56	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-78.12	25.56	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-66.01	2.32	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-32.28	14.63	46.91	CaAl2O4
CaAl2O4:10H2O	-23.37	14.63	37.99	CaAl2O4:10H2O

CaAl4O7	-42.98	25.61	68.59	CaAl4O7
Carnallite	-19.54	-15.27	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.57	-5.10	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.49	-6.12	-2.63	CuSO4:5H2O
Chalcocyanite	-9.03	-6.12	2.91	CuSO4
Chloromagnesite	-31.28	-9.47	21.82	MgCl2
Cl2(g)	-27.91	-24.92	2.99	Cl2
Claudetite	-30.88	-50.68	-19.80	As2O3
Corundum	-7.31	10.98	18.29	Al2O3
Cu	-16.21	15.29	31.50	Cu
Cu(g)	-68.37	15.29	83.66	Cu
CuCl2	-13.35	-9.63	3.72	CuCl2
Cuprite	-17.69	-19.60	-1.91	Cu2O
Delafossite	1.85	-4.59	-6.44	CuFeO2
Diaspore	-1.66	5.49	7.15	AlHO2
Epsomite	-3.99	-5.95	-1.96	MgSO4:7H2O
Ettringite	-55.86	6.60	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-43.30	15.72	59.02	Fe
Fe(OH)2	-10.83	3.06	13.89	Fe(OH)2
Fe(OH)3	-0.43	5.21	5.64	Fe(OH)3
Fe2(SO4)3	-18.86	-15.82	3.05	Fe2(SO4)3
FeO	-10.46	3.06	13.52	FeO
Ferrite-Ca	-7.42	14.07	21.50	CaFe2O4
Ferrite-Cu	2.78	13.06	10.28	CuFe2O4
Ferrite-Dicalcium	-39.08	17.72	56.80	Ca2Fe2O5
Ferrite-Mg	-7.80	13.22	21.02	MgFe2O4
Ferrite-Zn	1.05	12.75	11.70	ZnFe2O4
FeSO4	-8.29	-5.69	2.61	FeSO4
Gibbsite	-2.25	5.49	7.74	Al(OH)3
Glauberite	-7.90	-13.37	-5.47	Na2Ca(SO4)2
Goethite	4.68	5.21	0.53	FeOOH
Gypsum	-0.57	-5.10	-4.53	CaSO4:2H2O
H2(g)	-30.34	-33.44	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.45	-5.89	1.56	NaCl
Hausmannite	-23.59	-13.45	10.14	Mn3O4
HCl(g)	-12.43	-6.13	6.30	HCl
Hematite	10.35	10.43	0.08	Fe2O3
Hercynite	-14.76	14.04	28.80	FeAl2O4
Hexahydrite	-4.23	-5.95	-1.73	MgSO4:6H2O
Hydrophilite	-20.36	-8.62	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.88	-1.53	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.84	-1.61	-5.45	NaFe3(SO4)2(OH)6
K	-64.32	6.65	70.98	K
K(g)	-74.93	6.65	81.58	K
K2O	-83.39	0.65	84.04	K2O
K3H(SO4)2	-12.90	-16.52	-3.62	K3H(SO4)2
Kainite	-11.45	-11.76	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-14.95	-11.68	3.27	KAl(SO4)2
Katoite	-57.03	21.91	78.94	Ca3Al2H12O12
Kieserite	-5.69	-5.95	-0.27	MgSO4:H2O
KMgCl3	-36.52	-15.27	21.25	KMgCl3
KMgCl3:2H2O	-29.23	-15.27	13.96	KMgCl3:2H2O
Lammerite	-8.58	-7.03	1.55	Cu3(AsO4)2
Lawrencite	-18.25	-9.20	9.05	FeCl2
Leonite	-9.94	-14.05	-4.11	K2Mg(SO4)2:4H2O
Lime	-28.92	3.64	32.57	CaO
Magnetite	3.07	13.49	10.42	Fe3O4
Manganite	-7.79	-7.95	-0.16	MnO(OH)
Manganosite	-15.46	2.45	17.92	MnO
Mayenite	-373.54	120.61	494.15	Ca12Al14O33
Melanterite	-3.29	-5.69	-2.40	FeSO4:7H2O
Mercallite	-6.99	-8.42	-1.44	KHSO4
Mg	-107.07	15.45	122.52	Mg
Mg(g)	-126.79	15.45	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.45	-5.25	5.20	Mg1.25SO4(OH)0.5:0.5H2O

Mg1.5SO4(OH)	-13.77	-4.56	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.20	-9.47	12.73	MgCl2:2H2O
MgCl2:4H2O	-16.77	-9.47	7.30	MgCl2:4H2O
MgCl2:H2O	-25.54	-9.47	16.07	MgCl2:H2O
MgOHCl	-19.23	-3.34	15.89	MgOHCl
MgSO4	-10.78	-5.95	4.83	MgSO4
Mirabilite	-7.11	-8.27	-1.15	Na2SO4:10H2O
Misenite	-47.57	-58.64	-11.08	K8H6(SO4)7
Mn	-67.82	15.11	82.93	Mn
Mn(OH)2(am)	-12.85	2.45	15.31	Mn(OH)2
Mn(OH)3	-14.29	-7.95	6.34	Mn(OH)3
MnCl2:2H2O	-13.80	-9.81	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.56	-9.81	2.75	MnCl2:4H2O
MnCl2:H2O	-15.35	-9.81	5.54	MnCl2:H2O
MnO2(gamma)	-10.30	-26.43	-16.13	MnO2
MnSO4	-8.90	-6.29	2.61	MnSO4
Molysite	-26.65	-13.18	13.47	FeCl3
Na	-60.80	6.57	67.37	Na
Na(g)	-74.29	6.57	80.86	Na
Na2O	-66.93	0.48	67.42	Na2O
Na3H(SO4)2	-15.88	-16.77	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-15.74	-21.63	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.43	5.46	19.88	NaFeO2
Nantokite	-9.16	-15.93	-6.77	CuCl
O2(g)	-22.42	-25.32	-2.89	O2
Oxychloride-Mg	-26.37	-0.54	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.57	-5.95	-1.39	MgSO4:5H2O
Periclase	-18.53	2.79	21.33	MgO
Picromerite	-9.61	-14.05	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-9.95	-24.26	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-18.90	3.64	22.55	Ca(OH)2
Pyrolusite	-8.77	-26.43	-17.66	MnO2
Scacchite	-18.55	-9.81	8.74	MnCl2
Spinel	-23.83	13.78	37.61	Al2MgO4
Starkeyite	-4.95	-5.95	-1.00	MgSO4:4H2O
Sylvite	-6.63	-5.81	0.83	KCl
Syngenite	-5.60	-13.20	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-44.69	-27.55	17.14	Mg2CaCl6:12H2O
Tenorite	-5.01	2.63	7.65	CuO
Thenardite	-7.91	-8.26	-0.36	Na2SO4
Todorokite	-57.19	-103.02	-45.82	Mn7O12:3H2O
Wustite	-9.27	3.13	12.40	Fe.947O
Zincite	-8.87	2.33	11.20	ZnO
Zn	-53.80	14.98	68.79	Zn
Zn(ClO4)2:6H2O	-148.28	-142.65	5.63	Zn(ClO4)2:6H2O
Zn(g)	-70.42	14.98	85.41	Zn
Zn(OH)2(beta)	-9.61	2.33	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.33	2.33	11.66	Zn(OH)2
Zn(OH)2(gamma)	-9.56	2.33	11.88	Zn(OH)2
Zn2(OH)3Cl	-16.77	-1.48	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-11.68	-4.09	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-17.26	-7.95	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-29.61	-10.52	19.09	Zn3O(SO4)2
ZnCl2	-17.01	-9.93	7.08	ZnCl2
ZnSO4	-9.95	-6.42	3.53	ZnSO4
ZnSO4:6H2O	-4.72	-6.42	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.54	-6.42	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-5.87	-6.42	-0.55	ZnSO4:H2O

Initial solution 4. AS3

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

Elements	Molality	Moles
As	1.290e-006	1.290e-006
C(4)	1.901e-003	1.901e-003

Ca	2.167e-003	2.167e-003
Cl	6.830e-004	6.830e-004
Cu	1.779e-006	1.779e-006
K	7.856e-005	7.856e-005
Mg	6.656e-004	6.656e-004
Mn	3.296e-006	3.296e-006
Na	1.872e-003	1.872e-003
S(6)	2.531e-003	2.531e-003
Zn	2.984e-006	2.984e-006

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

pH	=	7.740
pe	=	10.000
Activity of water	=	1.000
Ionic strength	=	1.132e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	1.857e-003
Total CO2 (mol/kg)	=	1.901e-003
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	2.892e-005
Percent error, 100*(Cat- An )/(Cat+ An )	=	0.21
Iterations	=	4
Total H	=	1.110525e+002
Total O	=	5.554109e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.913e-007	5.294e-007	-6.228	-6.276	-0.048
H+	1.999e-008	1.820e-008	-7.699	-7.740	-0.041
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-139.943	-139.943	0.000
As(3)	5.393e-029				
HAsO2	2.782e-029	2.782e-029	-28.556	-28.556	0.000
As(OH)3	2.432e-029	2.432e-029	-28.614	-28.614	0.000
H2AsO3-	9.114e-031	8.174e-031	-30.040	-30.088	-0.047
AsO2-	8.714e-031	7.815e-031	-30.060	-30.107	-0.047
AsO2OH-2	6.804e-034	4.389e-034	-33.167	-33.358	-0.190
As(5)	1.290e-006				
HAsO4-2	1.195e-006	7.711e-007	-5.922	-6.113	-0.190
H2AsO4-	9.424e-008	8.452e-008	-7.026	-7.073	-0.047
AsO4-3	2.920e-010	1.087e-010	-9.535	-9.964	-0.429
H3AsO4	2.709e-013	2.709e-013	-12.567	-12.567	0.000
C(4)	1.901e-003				
HCO3-	1.776e-003	1.593e-003	-2.751	-2.798	-0.047
CO2	6.706e-005	6.724e-005	-4.174	-4.172	0.001
CaHCO3+	2.618e-005	2.348e-005	-4.582	-4.629	-0.047
CaCO3	1.119e-005	1.119e-005	-4.951	-4.951	0.000
MgHCO3+	7.342e-006	6.584e-006	-5.134	-5.181	-0.047
CO3-2	5.981e-006	3.883e-006	-5.223	-5.411	-0.188
NaHCO3	3.782e-006	3.782e-006	-5.422	-5.422	0.000
CuCO3	1.553e-006	1.553e-006	-5.809	-5.809	0.000
MgCO3	1.462e-006	1.462e-006	-5.835	-5.835	0.000
MnCO3	2.237e-007	2.237e-007	-6.650	-6.650	0.000
ZnHCO3+	6.961e-008	6.243e-008	-7.157	-7.205	-0.047
ZnCO3	4.958e-008	4.958e-008	-7.305	-7.305	0.000
NaCO3-	2.515e-008	2.256e-008	-7.599	-7.647	-0.047
MnHCO3+	2.225e-008	1.996e-008	-7.653	-7.700	-0.047
Cu(CO3)2-2	1.666e-008	1.075e-008	-7.778	-7.969	-0.190
CuCO3(OH)2-2	6.181e-011	3.987e-011	-10.209	-10.399	-0.190
Ca	2.167e-003				
Ca+2	1.880e-003	1.244e-003	-2.726	-2.905	-0.179
CaSO4	2.499e-004	2.499e-004	-3.602	-3.602	0.000

CaHCO <sub>3</sub> <sup>+</sup>	2.618e-005	2.348e-005	-4.582	-4.629	-0.047
CaCO <sub>3</sub>	1.119e-005	1.119e-005	-4.951	-4.951	0.000
CaCl <sup>+</sup>	1.793e-007	1.608e-007	-6.746	-6.794	-0.047
CaOH <sup>+</sup>	1.076e-008	9.653e-009	-7.968	-8.015	-0.047
CaCl <sub>2</sub>	1.153e-010	1.153e-010	-9.938	-9.938	0.000
Cl(-1)	6.830e-004				
Cl <sup>-</sup>	6.824e-004	6.099e-004	-3.166	-3.215	-0.049
MgCl <sup>+</sup>	1.890e-007	1.695e-007	-6.724	-6.771	-0.047
CaCl <sup>+</sup>	1.793e-007	1.608e-007	-6.746	-6.794	-0.047
NaCl	1.780e-007	1.780e-007	-6.750	-6.750	0.000
MnCl <sup>+</sup>	2.383e-009	2.137e-009	-8.623	-8.670	-0.047
ZnCl <sup>+</sup>	1.737e-009	1.558e-009	-8.760	-8.807	-0.047
Zn(OH)Cl	1.464e-009	1.464e-009	-8.835	-8.835	0.000
KCl	1.422e-009	1.422e-009	-8.847	-8.847	0.000
CaCl <sub>2</sub>	1.153e-010	1.153e-010	-9.938	-9.938	0.000
CuCl <sup>+</sup>	7.800e-011	6.996e-011	-10.108	-10.155	-0.047
HCl	2.493e-012	2.493e-012	-11.603	-11.603	0.000
ZnCl <sub>2</sub>	1.110e-012	1.110e-012	-11.955	-11.955	0.000
CuCl <sub>2</sub>	2.247e-014	2.247e-014	-13.648	-13.648	0.000
ZnCl <sub>3</sub> <sup>-</sup>	4.169e-016	3.739e-016	-15.380	-15.427	-0.047
MnCl <sub>3</sub> <sup>-</sup>	1.936e-016	1.737e-016	-15.713	-15.760	-0.047
CuCl <sub>2</sub> <sup>-</sup>	6.308e-017	5.658e-017	-16.200	-16.247	-0.047
ZnCl <sub>4</sub> <sup>-2</sup>	2.680e-018	1.729e-018	-17.572	-17.762	-0.190
CuCl <sub>3</sub> <sup>-2</sup>	3.436e-019	2.216e-019	-18.464	-18.654	-0.190
CuCl <sub>4</sub> <sup>-2</sup>	2.432e-025	1.569e-025	-24.614	-24.804	-0.190
Cl(1)	2.568e-026				
ClO <sup>-</sup>	1.599e-026	1.435e-026	-25.796	-25.843	-0.047
HClO	9.681e-027	9.681e-027	-26.014	-26.014	0.000
Cl(3)	0.000e+000				
ClO <sub>2</sub> <sup>-</sup>	0.000e+000	0.000e+000	-41.319	-41.366	-0.047
HClO <sub>2</sub>	0.000e+000	0.000e+000	-45.937	-45.937	0.000
Cl(5)	0.000e+000				
ClO <sub>3</sub> <sup>-</sup>	0.000e+000	0.000e+000	-42.989	-43.037	-0.048
Cl(7)	0.000e+000				
ClO <sub>4</sub> <sup>-</sup>	0.000e+000	0.000e+000	-48.962	-49.010	-0.048
ZnClO <sub>4</sub> <sup>+</sup>	0.000e+000	0.000e+000	-53.504	-53.551	-0.047
Cu(1)	2.623e-015				
Cu <sup>+</sup>	2.560e-015	2.296e-015	-14.592	-14.639	-0.047
CuCl <sub>2</sub> <sup>-</sup>	6.308e-017	5.658e-017	-16.200	-16.247	-0.047
CuCl <sub>3</sub> <sup>-2</sup>	3.436e-019	2.216e-019	-18.464	-18.654	-0.190
Cu(2)	1.779e-006				
CuCO <sub>3</sub>	1.553e-006	1.553e-006	-5.809	-5.809	0.000
CuOH <sup>+</sup>	1.325e-007	1.189e-007	-6.878	-6.925	-0.047
Cu <sup>2</sup>	6.339e-008	4.193e-008	-7.198	-7.377	-0.179
Cu(CO <sub>3</sub> ) <sub>2</sub> <sup>-2</sup>	1.666e-008	1.075e-008	-7.778	-7.969	-0.190
CuSO <sub>4</sub>	1.321e-008	1.321e-008	-7.879	-7.879	0.000
CuCl <sup>+</sup>	7.800e-011	6.996e-011	-10.108	-10.155	-0.047
CuCO <sub>3</sub> (OH) <sub>2</sub> <sup>-2</sup>	6.181e-011	3.987e-011	-10.209	-10.399	-0.190
CuCl <sub>2</sub>	2.247e-014	2.247e-014	-13.648	-13.648	0.000
CuO <sub>2</sub> <sup>-2</sup>	2.105e-016	1.357e-016	-15.677	-15.867	-0.190
CuCl <sub>4</sub> <sup>-2</sup>	2.432e-025	1.569e-025	-24.614	-24.804	-0.190
H(0)	5.241e-039				
H <sub>2</sub>	2.620e-039	2.628e-039	-38.582	-38.580	0.001
K	7.856e-005				
K <sup>+</sup>	7.770e-005	6.945e-005	-4.110	-4.158	-0.049
KSO <sub>4</sub> <sup>-</sup>	8.595e-007	7.709e-007	-6.066	-6.113	-0.047
KCl	1.422e-009	1.422e-009	-8.847	-8.847	0.000
KOH	1.323e-011	1.323e-011	-10.878	-10.878	0.000
KHSO <sub>4</sub>	1.238e-014	1.238e-014	-13.907	-13.907	0.000
Mg	6.656e-004				
Mg <sup>2</sup>	5.259e-004	3.559e-004	-3.279	-3.449	-0.170
MgSO <sub>4</sub>	1.307e-004	1.307e-004	-3.884	-3.884	0.000
MgHCO <sub>3</sub> <sup>+</sup>	7.342e-006	6.584e-006	-5.134	-5.181	-0.047
MgCO <sub>3</sub>	1.462e-006	1.462e-006	-5.835	-5.835	0.000
MgCl <sup>+</sup>	1.890e-007	1.695e-007	-6.724	-6.771	-0.047
Mg <sub>4</sub> (OH) <sub>4</sub> <sup>4+</sup>	1.396e-022	2.601e-023	-21.855	-22.585	-0.730
Mn(2)	3.296e-006				

Mn+2	2.487e-006	1.645e-006	-5.604	-5.784	-0.179
MnSO4	5.583e-007	5.583e-007	-6.253	-6.253	0.000
MnCO3	2.237e-007	2.237e-007	-6.650	-6.650	0.000
MnHCO3+	2.225e-008	1.996e-008	-7.653	-7.700	-0.047
MnOH+	2.591e-009	2.324e-009	-8.587	-8.634	-0.047
MnCl+	2.383e-009	2.137e-009	-8.623	-8.670	-0.047
Mn2(OH)3+	6.304e-013	5.654e-013	-12.200	-12.248	-0.047
Mn(OH)2	3.134e-013	3.134e-013	-12.504	-12.504	0.000
Mn2OH+3	1.069e-014	4.097e-015	-13.971	-14.388	-0.416
MnCl3-	1.936e-016	1.737e-016	-15.713	-15.760	-0.047
Mn(OH)3-	1.801e-017	1.615e-017	-16.744	-16.792	-0.047
Mn(OH)4-2	1.165e-023	7.516e-024	-22.934	-23.124	-0.190
Mn(3)	1.145e-021				
Mn+3	1.145e-021	4.389e-022	-20.941	-21.358	-0.416
Mn(6)	7.578e-023				
MnO4-2	7.578e-023	4.888e-023	-22.120	-22.311	-0.190
Mn(7)	2.404e-022				
MnO4-	2.404e-022	2.152e-022	-21.619	-21.667	-0.048
Na	1.872e-003				
Na+	1.851e-003	1.660e-003	-2.733	-2.780	-0.047
NaSO4-	1.682e-005	1.508e-005	-4.774	-4.821	-0.047
NaHCO3	3.782e-006	3.782e-006	-5.422	-5.422	0.000
NaCl	1.780e-007	1.780e-007	-6.750	-6.750	0.000
NaCO3-	2.515e-008	2.256e-008	-7.599	-7.647	-0.047
NaOH	1.516e-010	1.516e-010	-9.819	-9.819	0.000
O(0)	1.839e-015				
O2	9.196e-016	9.221e-016	-15.036	-15.035	0.001
S(6)	2.531e-003				
SO4-2	2.132e-003	1.375e-003	-2.671	-2.862	-0.190
CaSO4	2.499e-004	2.499e-004	-3.602	-3.602	0.000
MgSO4	1.307e-004	1.307e-004	-3.884	-3.884	0.000
NaSO4-	1.682e-005	1.508e-005	-4.774	-4.821	-0.047
KSO4-	8.595e-007	7.709e-007	-6.066	-6.113	-0.047
MnSO4	5.583e-007	5.583e-007	-6.253	-6.253	0.000
ZnSO4	4.394e-007	4.394e-007	-6.357	-6.357	0.000
CuSO4	1.321e-008	1.321e-008	-7.879	-7.879	0.000
HSO4-	2.818e-009	2.528e-009	-8.550	-8.597	-0.047
KHSO4	1.238e-014	1.238e-014	-13.907	-13.907	0.000
H2SO4	4.340e-020	4.340e-020	-19.363	-19.363	0.000
Zn	2.984e-006				
Zn+2	2.298e-006	1.520e-006	-5.639	-5.818	-0.179
ZnSO4	4.394e-007	4.394e-007	-6.357	-6.357	0.000
ZnOH+	1.022e-007	9.162e-008	-6.991	-7.038	-0.047
ZnHCO3+	6.961e-008	6.243e-008	-7.157	-7.205	-0.047
ZnCO3	4.958e-008	4.958e-008	-7.305	-7.305	0.000
Zn(OH)2	2.156e-008	2.156e-008	-7.666	-7.666	0.000
ZnCl+	1.737e-009	1.558e-009	-8.760	-8.807	-0.047
Zn(OH)Cl	1.464e-009	1.464e-009	-8.835	-8.835	0.000
Zn(OH)3-	4.094e-012	3.672e-012	-11.388	-11.435	-0.047
ZnCl2	1.110e-012	1.110e-012	-11.955	-11.955	0.000
ZnCl3-	4.169e-016	3.739e-016	-15.380	-15.427	-0.047
Zn(OH)4-2	5.333e-017	3.439e-017	-16.273	-16.464	-0.190
ZnCl4-2	2.680e-018	1.729e-018	-17.572	-17.762	-0.190
ZnClO4+	0.000e+000	0.000e+000	-53.504	-53.551	-0.047

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

Phase	SI	log IAP	log KT	
Anhydrite	-1.42	-5.77	-4.35	CaSO4
Antarcticite	-13.43	-9.34	4.09	CaCl2:6H2O
Antlerite	-2.76	5.97	8.73	Cu3(SO4)(OH)4
Aphthitalite	-17.09	-20.98	-3.89	NaK3(SO4)2
Aragonite	0.07	2.04	1.97	CaCO3
Arcanite	-9.33	-11.18	-1.84	K2SO4
Arsenolite	-55.81	-75.65	-19.84	As2O3
Artinite	-6.10	13.52	19.63	Mg2CO3(OH)2:3H2O

As	-69.23	-26.55	42.68	As
As2O5	-31.76	-29.63	2.14	As2O5
As4O6(cubi)	-111.49	-151.31	-39.82	As4O6
As4O6(mono)	-111.26	-151.31	-40.05	As4O6
Atacamite	-3.76	10.50	14.26	Cu4Cl2(OH)6
Azurite	-5.88	3.23	9.12	Cu3(CO3)2(OH)2
Bassanite	-2.06	-5.77	-3.71	CaSO4:0.5H2O
Birnessite	20.65	-64.89	-85.55	Mn8O14:5H2O
Bischofite	-14.27	-9.88	4.39	MgCl2:6H2O
Bixbyite	4.69	3.72	-0.96	Mn2O3
Bloedite	-12.25	-14.73	-2.48	Na2Mg(SO4)2:4H2O
Brochantite	-1.35	14.07	15.42	Cu4(SO4)(OH)6
Brucite	-4.25	12.03	16.28	Mg(OH)2
Burkeite	-26.95	-17.46	9.49	Na6CO3(SO4)2
C	-59.65	4.50	64.15	C
C(g)	-177.27	4.50	181.77	C
Ca	-119.74	20.09	139.83	Ca
Ca(g)	-144.98	20.09	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.05	3.24	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-9.70	8.10	17.80	Ca3(AsO4)2
Ca4Cl2(OH)6:13H2O	-39.94	28.39	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.21	2.04	1.82	CaCO3
Carnallite	-21.52	-17.25	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.23	-5.77	-3.54	CaSO4:0.5H2O
Chalcanthite	-7.61	-10.24	-2.63	CuSO4:5H2O
Chalcocyanite	-13.15	-10.24	2.91	CuSO4
Chloromagnesite	-31.69	-9.88	21.82	MgCl2
Cl2(g)	-32.42	-29.43	2.99	Cl2
Claudetite	-55.86	-75.65	-19.80	As2O3
CO2(g)	-2.71	-10.54	-7.83	CO2
Cu	-15.88	15.62	31.50	Cu
Cu(g)	-68.04	15.62	83.66	Cu
CuCl2	-17.53	-13.81	3.72	CuCl2
Cuprite	-11.89	-13.80	-1.91	Cu2O
Dolomite	1.06	3.53	2.47	CaMg(CO3)2
Dolomite-dis	-0.48	3.53	4.01	CaMg(CO3)2
Dolomite-ord	1.07	3.53	2.46	CaMg(CO3)2
Epsomite	-4.35	-6.31	-1.96	MgSO4:7H2O
Gaylussite	-9.75	1.42	11.16	CaNa2(CO3)2:5H2O
Glauberite	-8.72	-14.19	-5.47	Na2Ca(SO4)2
Gypsum	-1.24	-5.77	-4.53	CaSO4:2H2O
H2(g)	-35.48	-38.58	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.56	-5.99	1.56	NaCl
Hausmannite	3.28	13.42	10.14	Mn3O4
HCl(g)	-17.26	-10.95	6.30	HCl
Hexahydrate	-4.58	-6.31	-1.73	MgSO4:6H2O
Huntite	-3.70	6.52	10.22	CaMg3(CO3)4
Hydromagnesite	-12.73	18.01	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.08	-9.33	11.75	CaCl2
Hydrozincite	-3.07	27.23	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
K	-63.64	7.34	70.98	K
K(g)	-74.24	7.34	81.58	K
K2CO3:1.5H2O	-16.75	-3.37	13.38	K2CO3:1.5H2O
K2O	-76.87	7.16	84.04	K2O
K3H(SO4)2	-22.32	-25.94	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-62.28	-34.57	27.71	K8H4(CO3)6:3H2O
Kainite	-13.37	-13.68	-0.31	KMgClSO4:3H2O
Kaliginite	-7.24	-6.96	0.28	KHCO3
Kieserite	-6.04	-6.31	-0.27	MgSO4:H2O
KMgCl3	-38.50	-17.25	21.25	KMgCl3
KMgCl3:2H2O	-31.21	-17.25	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-12.26	-2.00	10.26	KNaCO3:6H2O
Lammerite	-6.87	-5.32	1.55	Cu3(AsO4)2
Lansfordite	-3.35	1.49	4.84	MgCO3:5H2O
Leonite	-13.38	-17.49	-4.11	K2Mg(SO4)2:4H2O

Lime	-19.99	12.57	32.57	CaO
Magnesite	-0.78	1.49	2.27	MgCO <sub>3</sub>
Malachite	-0.23	5.67	5.90	Cu <sub>2</sub> CO <sub>3</sub> (OH) <sub>2</sub>
Manganite	2.03	1.86	-0.16	MnO(OH)
Manganosite	-8.22	9.70	17.92	MnO
Mercallite	-13.32	-14.76	-1.44	KHSO <sub>4</sub>
Mg	-102.97	19.55	122.52	Mg
Mg(g)	-122.70	19.55	142.25	Mg
Mg1.25SO <sub>4</sub> (OH)0.5:0.5H <sub>2</sub> O	-8.50	-3.30	5.20	Mg1.25SO <sub>4</sub> (OH)0.5:0.5H <sub>2</sub> O
Mg1.5SO <sub>4</sub> (OH)	-9.50	-0.29	9.21	Mg1.5SO <sub>4</sub> (OH)
MgCl <sub>2</sub> :2H <sub>2</sub> O	-22.61	-9.88	12.73	MgCl <sub>2</sub> :2H <sub>2</sub> O
MgCl <sub>2</sub> :4H <sub>2</sub> O	-17.18	-9.88	7.30	MgCl <sub>2</sub> :4H <sub>2</sub> O
MgCl <sub>2</sub> :H <sub>2</sub> O	-25.95	-9.88	16.07	MgCl <sub>2</sub> :H <sub>2</sub> O
MgOHCl	-14.81	1.08	15.89	MgOHCl
MgSO <sub>4</sub>	-11.14	-6.31	4.83	MgSO <sub>4</sub>
Mirabilite	-7.27	-8.42	-1.15	Na <sub>2</sub> SO <sub>4</sub> :10H <sub>2</sub> O
Misenite	-88.66	-99.74	-11.08	K <sub>8</sub> H <sub>6</sub> (SO <sub>4</sub> ) <sub>7</sub>
Mn	-65.72	17.21	82.93	Mn
Mn(OH) <sub>2</sub> (am)	-5.61	9.70	15.31	Mn(OH) <sub>2</sub>
Mn(OH) <sub>3</sub>	-4.48	1.86	6.34	Mn(OH) <sub>3</sub>
MnCl <sub>2</sub> :2H <sub>2</sub> O	-16.21	-12.21	4.00	MnCl <sub>2</sub> :2H <sub>2</sub> O
MnCl <sub>2</sub> :4H <sub>2</sub> O	-14.97	-12.21	2.75	MnCl <sub>2</sub> :4H <sub>2</sub> O
MnCl <sub>2</sub> :H <sub>2</sub> O	-17.76	-12.21	5.54	MnCl <sub>2</sub> :H <sub>2</sub> O
MnO <sub>2</sub> (gamma)	2.08	-14.05	-16.13	MnO <sub>2</sub>
MnSO <sub>4</sub>	-11.25	-8.65	2.61	MnSO <sub>4</sub>
Monohydrocalcite	-0.64	2.04	2.68	CaCO <sub>3</sub> :H <sub>2</sub> O
Na	-58.65	8.72	67.37	Na
Na(g)	-72.14	8.72	80.86	Na
Na <sub>2</sub> CO <sub>3</sub>	-11.78	-0.62	11.16	Na <sub>2</sub> CO <sub>3</sub>
Na <sub>2</sub> CO <sub>3</sub> :7H <sub>2</sub> O	-10.56	-0.62	9.94	Na <sub>2</sub> CO <sub>3</sub> :7H <sub>2</sub> O
Na <sub>2</sub> O	-57.50	9.92	67.42	Na <sub>2</sub> O
Na <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>	-20.91	-21.80	-0.89	Na <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>
Na <sub>4</sub> Ca(SO <sub>4</sub> ) <sub>3</sub> :2H <sub>2</sub> O	-16.72	-22.61	-5.89	Na <sub>4</sub> Ca(SO <sub>4</sub> ) <sub>3</sub> :2H <sub>2</sub> O
Nahcolite	-5.44	-5.58	-0.14	NaHCO <sub>3</sub>
Nantokite	-11.09	-17.85	-6.77	CuCl
Natron	-10.21	-0.62	9.59	Na <sub>2</sub> CO <sub>3</sub> :10H <sub>2</sub> O
Nesquehonite	-3.80	1.49	5.29	MgCO <sub>3</sub> :3H <sub>2</sub> O
O <sub>2</sub> (g)	-12.14	-15.04	-2.89	O <sub>2</sub>
Oxychloride-Mg	-12.72	13.11	25.83	Mg <sub>2</sub> Cl(OH) <sub>3</sub> :4H <sub>2</sub> O
Pentahydrate	-4.92	-6.31	-1.39	MgSO <sub>4</sub> :5H <sub>2</sub> O
Periclase	-9.29	12.03	21.33	MgO
Picromerite	-13.05	-17.49	-4.44	K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> :6H <sub>2</sub> O
Pirssonite	-9.90	1.42	11.32	Na <sub>2</sub> Ca(CO <sub>3</sub> ) <sub>2</sub> :2H <sub>2</sub> O
Polyhalite	-14.71	-29.02	-14.31	K <sub>2</sub> MgCa <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub> :2H <sub>2</sub> O
Portlandite	-9.97	12.57	22.55	Ca(OH) <sub>2</sub>
Pyrolusite	3.61	-14.05	-17.66	MnO <sub>2</sub>
Rhodochrosite	-0.62	-0.84	-0.22	MnCO <sub>3</sub>
Scacchite	-20.95	-12.21	8.74	MnCl <sub>2</sub>
Smithsonite	-1.32	-0.88	0.44	ZnCO <sub>3</sub>
Starkeyite	-5.31	-6.31	-1.00	MgSO <sub>4</sub> :4H <sub>2</sub> O
Sylvite	-8.20	-7.37	0.83	KCl
Syngenite	-9.35	-16.95	-7.60	K <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub> :H <sub>2</sub> O
Tachyhydrate	-46.24	-29.09	17.14	Mg <sub>2</sub> CaCl <sub>6</sub> :12H <sub>2</sub> O
Tenorite	0.46	8.10	7.65	CuO
Thenardite	-8.06	-8.42	-0.36	Na <sub>2</sub> SO <sub>4</sub>
Thermonatrite	-11.55	-0.62	10.94	Na <sub>2</sub> CO <sub>3</sub> :H <sub>2</sub> O
Todorokite	19.21	-26.62	-45.82	Mn <sub>7</sub> O <sub>12</sub> :3H <sub>2</sub> O
Trona-K	-20.54	-8.95	11.59	K <sub>2</sub> NaH(CO <sub>3</sub> ) <sub>2</sub> :2H <sub>2</sub> O
Zincite	-1.54	9.66	11.20	ZnO
Zn	-51.61	17.18	68.79	Zn
Zn(ClO <sub>4</sub> ) <sub>2</sub> :6H <sub>2</sub> O	-109.47	-103.84	5.63	Zn(ClO <sub>4</sub> ) <sub>2</sub> :6H <sub>2</sub> O
Zn(g)	-68.23	17.18	85.41	Zn
Zn(OH) <sub>2</sub> (beta)	-2.27	9.66	11.93	Zn(OH) <sub>2</sub>
Zn(OH) <sub>2</sub> (epsilon)	-2.00	9.66	11.66	Zn(OH) <sub>2</sub>
Zn(OH) <sub>2</sub> (gamma)	-2.22	9.66	11.88	Zn(OH) <sub>2</sub>
Zn <sub>2</sub> (OH) <sub>3</sub> Cl	-6.92	8.37	15.29	Zn <sub>2</sub> (OH) <sub>3</sub> Cl
Zn <sub>2</sub> SO <sub>4</sub> (OH) <sub>2</sub>	-6.60	0.98	7.58	Zn <sub>2</sub> SO <sub>4</sub> (OH) <sub>2</sub>

Zn3(AsO4)2	-9.95	-0.64	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-26.79	-7.70	19.09	Zn3O(SO4)2
ZnCl2	-19.33	-12.25	7.08	ZnCl2
ZnCO3:H2O	-1.02	-0.88	0.14	ZnCO3:H2O
ZnSO4	-12.21	-8.68	3.53	ZnSO4
ZnSO4:6H2O	-6.98	-8.68	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-6.80	-8.68	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-8.13	-8.68	-0.55	ZnSO4:H2O

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

Reaction step 1.

Using mix 4.

Mixture 4.

1.000e+000 Solution 1 Flujo 4  
1.000e+000 Solution 4 AS3

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

Elements	Molality	Moles
Al	4.752e-004	9.504e-004
As	3.407e-005	6.814e-005
C	9.505e-004	1.901e-003
Ca	3.601e-003	7.201e-003
Cl	1.004e-003	2.008e-003
Cu	2.775e-004	5.551e-004
Fe	1.526e-003	3.053e-003
K	9.258e-004	1.852e-003
Mg	7.409e-004	1.482e-003
Mn	1.895e-004	3.789e-004
Na	1.659e-003	3.318e-003
S	6.948e-003	1.390e-002
Zn	1.348e-004	2.695e-004

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

pH	=	3.988	Charge balance
pe	=	10.911	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	2.312e-002	
Mass of water (kg)	=	2.000e+000	
Total alkalinity (eq/kg)	=	-4.308e-004	
Total CO2 (mol/kg)	=	9.505e-004	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	3.183e-003	
Percent error, 100*(Cat- An )/(Cat+ An )	=	6.35	
Iterations	=	14	
Total H	=	2.221062e+002	
Total O	=	1.111139e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.161e-004	1.029e-004	-3.935	-3.988	-0.053
OH-	1.088e-010	9.365e-011	-9.963	-10.028	-0.065
H2O	5.553e+001	9.997e-001	1.744	-0.000	0.000
Al	4.752e-004				
AlSO4+	2.199e-004	1.898e-004	-3.658	-3.722	-0.064
Al+3	1.929e-004	6.362e-005	-3.715	-4.196	-0.482

Al(SO <sub>4</sub> ) <sub>2</sub> -	4.976e-005	4.296e-005	-4.303	-4.367	-0.064
AlOH+2	1.240e-005	6.927e-006	-4.906	-5.159	-0.253
Al(OH) <sub>2</sub> +	1.811e-007	1.563e-007	-6.742	-6.806	-0.064
Al <sub>2</sub> (OH) <sub>2</sub> +4	7.364e-008	7.803e-009	-7.133	-8.108	-0.975
HALO <sub>2</sub>	2.212e-009	2.212e-009	-8.655	-8.655	0.000
Al <sub>3</sub> (OH) <sub>4</sub> +5	9.451e-010	3.027e-011	-9.025	-10.519	-1.494
AlO <sub>2</sub> -	8.536e-012	7.369e-012	-11.069	-11.133	-0.064
NaAlO <sub>2</sub>	1.975e-015	1.975e-015	-14.704	-14.704	0.000
Al <sub>13</sub> O <sub>4</sub> (OH) <sub>24</sub> +7	1.787e-023	2.100e-026	-22.748	-25.678	-2.930
As(-3)	0.000e+000				
AsH <sub>3</sub>	0.000e+000	0.000e+000	-110.929	-110.929	0.000
As(3)	4.845e-017				
HAsO <sub>2</sub>	2.585e-017	2.585e-017	-16.588	-16.588	0.000
As(OH) <sub>3</sub>	2.260e-017	2.260e-017	-16.646	-16.646	0.000
H <sub>2</sub> AsO <sub>3</sub> -	1.556e-022	1.344e-022	-21.808	-21.872	-0.064
AsO <sub>2</sub> -	1.488e-022	1.285e-022	-21.827	-21.891	-0.064
AsO <sub>2</sub> OH-2	2.313e-029	1.276e-029	-28.636	-28.894	-0.258
HAsS <sub>2</sub>	0.000e+000	0.000e+000	-187.368	-187.368	0.000
As(5)	3.407e-005				
H <sub>2</sub> AsO <sub>4</sub> -	3.346e-005	2.889e-005	-4.475	-4.539	-0.064
H <sub>3</sub> AsO <sub>4</sub>	5.233e-007	5.233e-007	-6.281	-6.281	0.000
HAsO <sub>4</sub> -2	8.450e-008	4.662e-008	-7.073	-7.331	-0.258
AsO <sub>4</sub> -3	4.444e-015	1.163e-015	-14.352	-14.934	-0.582
C(-2)	0.000e+000				
C <sub>2</sub> H <sub>4</sub>	0.000e+000	0.000e+000	-193.994	-193.994	0.000
C(-3)	0.000e+000				
C <sub>2</sub> H <sub>6</sub>	0.000e+000	0.000e+000	-154.905	-154.905	0.000
C(-4)	0.000e+000				
CH <sub>4</sub>	0.000e+000	0.000e+000	-100.680	-100.680	0.000
C(2)	1.375e-038				
CO	1.375e-038	1.375e-038	-37.862	-37.862	0.000
C(4)	9.505e-004				
CO <sub>2</sub>	9.450e-004	9.503e-004	-3.025	-3.022	0.002
HCO <sub>3</sub> -	4.613e-006	3.982e-006	-5.336	-5.400	-0.064
FeHCO <sub>3</sub> +	7.402e-007	6.390e-007	-6.131	-6.195	-0.064
CaHCO <sub>3</sub> +	9.124e-008	7.877e-008	-7.040	-7.104	-0.064
FeCO <sub>3</sub> +	2.746e-008	2.370e-008	-7.561	-7.625	-0.064
MgHCO <sub>3</sub> +	1.624e-008	1.402e-008	-7.789	-7.853	-0.064
NaHCO <sub>3</sub>	8.004e-009	8.004e-009	-8.097	-8.097	0.000
ZnHCO <sub>3</sub> +	6.832e-009	5.898e-009	-8.165	-8.229	-0.064
MnHCO <sub>3</sub> +	2.713e-009	2.342e-009	-8.567	-8.630	-0.064
CuCO <sub>3</sub>	1.893e-009	1.893e-009	-8.723	-8.723	0.000
FeCO <sub>3</sub>	2.982e-011	2.982e-011	-10.526	-10.526	0.000
CaCO <sub>3</sub>	6.645e-012	6.645e-012	-11.178	-11.178	0.000
MnCO <sub>3</sub>	4.645e-012	4.645e-012	-11.333	-11.333	0.000
CO <sub>3</sub> -2	3.076e-012	1.718e-012	-11.512	-11.765	-0.253
ZnCO <sub>3</sub>	8.289e-013	8.289e-013	-12.082	-12.082	0.000
MgCO <sub>3</sub>	5.509e-013	5.509e-013	-12.259	-12.259	0.000
NaCO <sub>3</sub> -	9.782e-015	8.445e-015	-14.010	-14.073	-0.064
Cu(CO <sub>3</sub> ) <sub>2</sub> -2	1.050e-017	5.792e-018	-16.979	-17.237	-0.258
CuCO <sub>3</sub> (OH) <sub>2</sub> -2	2.756e-021	1.520e-021	-20.560	-20.818	-0.258
Ca	3.601e-003				
Ca+2	2.889e-003	1.669e-003	-2.539	-2.778	-0.238
CaSO <sub>4</sub>	7.109e-004	7.109e-004	-3.148	-3.148	0.000
CaCl+	3.523e-007	3.042e-007	-6.453	-6.517	-0.064
CaHCO <sub>3</sub> +	9.124e-008	7.877e-008	-7.040	-7.104	-0.064
CaCl <sub>2</sub>	3.076e-010	3.076e-010	-9.512	-9.512	0.000
CaCO <sub>3</sub>	6.645e-012	6.645e-012	-11.178	-11.178	0.000
CaOH+	2.655e-012	2.292e-012	-11.576	-11.640	-0.064
Cl(-1)	1.004e-003				
Cl-	1.002e-003	8.598e-004	-2.999	-3.066	-0.067
CaCl+	3.523e-007	3.042e-007	-6.453	-6.517	-0.064
CuCl+	3.147e-007	2.717e-007	-6.502	-6.566	-0.064
MgCl+	2.357e-007	2.035e-007	-6.628	-6.691	-0.064
FeCl+	2.218e-007	1.915e-007	-6.654	-6.718	-0.064
NaCl	2.123e-007	2.123e-007	-6.673	-6.673	0.000
MnCl+	1.638e-007	1.414e-007	-6.786	-6.849	-0.064

ZnCl+	9.615e-008	8.300e-008	-7.017	-7.081	-0.064
KCl	2.240e-008	2.240e-008	-7.650	-7.650	0.000
HCl	1.986e-008	1.986e-008	-7.702	-7.702	0.000
FeCl+2	6.128e-010	3.423e-010	-9.213	-9.466	-0.253
CaCl2	3.076e-010	3.076e-010	-9.512	-9.512	0.000
FeCl2+	2.760e-010	2.383e-010	-9.559	-9.623	-0.064
CuCl2	1.230e-010	1.230e-010	-9.910	-9.910	0.000
ZnCl2	8.336e-011	8.336e-011	-10.079	-10.079	0.000
Zn(OH)Cl	1.379e-011	1.379e-011	-10.860	-10.860	0.000
FeCl2	8.835e-013	8.835e-013	-12.054	-12.054	0.000
ZnCl3-	4.585e-014	3.958e-014	-13.339	-13.403	-0.064
CuCl2-	4.402e-014	3.800e-014	-13.356	-13.420	-0.064
MnCl3-	2.645e-014	2.284e-014	-13.578	-13.641	-0.064
ZnCl4-2	4.675e-016	2.580e-016	-15.330	-15.588	-0.258
CuCl3-2	3.803e-016	2.098e-016	-15.420	-15.678	-0.258
FeCl4-2	3.421e-018	1.887e-018	-17.466	-17.724	-0.258
FeCl4-	2.453e-019	2.117e-019	-18.610	-18.674	-0.064
CuCl4-2	3.093e-021	1.707e-021	-20.510	-20.768	-0.258
Cl(1)	1.604e-028				
HClO	1.604e-028	1.604e-028	-27.795	-27.795	0.000
ClO-	4.871e-032	4.205e-032	-31.312	-31.376	-0.064
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-52.518	-52.582	-0.064
HClO2	0.000e+000	0.000e+000	-53.400	-53.400	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-59.869	-59.935	-0.065
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-71.524	-71.589	-0.065
ZnClO4+	0.000e+000	0.000e+000	-74.489	-74.553	-0.064
Cu(1)	9.433e-013				
Cu+	8.989e-013	7.760e-013	-12.046	-12.110	-0.064
CuCl2-	4.402e-014	3.800e-014	-13.356	-13.420	-0.064
CuCl3-2	3.803e-016	2.098e-016	-15.420	-15.678	-0.258
Cu(2)	2.775e-004				
Cu+2	2.000e-004	1.155e-004	-3.699	-3.937	-0.238
CuSO4	7.717e-005	7.717e-005	-4.113	-4.113	0.000
CuCl+	3.147e-007	2.717e-007	-6.502	-6.566	-0.064
CuOH+	6.710e-008	5.793e-008	-7.173	-7.237	-0.064
CuCO3	1.893e-009	1.893e-009	-8.723	-8.723	0.000
CuCl2	1.230e-010	1.230e-010	-9.910	-9.910	0.000
Cu(CO3)2-2	1.050e-017	5.792e-018	-16.979	-17.237	-0.258
CuCl4-2	3.093e-021	1.707e-021	-20.510	-20.768	-0.258
CuCO3(OH)2-2	2.756e-021	1.520e-021	-20.560	-20.818	-0.258
CuO2-2	6.640e-028	3.664e-028	-27.178	-27.436	-0.258
Fe(2)	6.715e-004				
Fe+2	5.293e-004	3.057e-004	-3.276	-3.515	-0.238
FeSO4	1.413e-004	1.413e-004	-3.850	-3.850	0.000
FeHCO3+	7.402e-007	6.390e-007	-6.131	-6.195	-0.064
FeCl+	2.218e-007	1.915e-007	-6.654	-6.718	-0.064
FeOH+	1.089e-009	9.398e-010	-8.963	-9.027	-0.064
FeCO3	2.982e-011	2.982e-011	-10.526	-10.526	0.000
FeCl2	8.835e-013	8.835e-013	-12.054	-12.054	0.000
Fe(OH)2	7.256e-017	7.256e-017	-16.139	-16.139	0.000
FeCl4-2	3.421e-018	1.887e-018	-17.466	-17.724	-0.258
Fe(OH)3-	3.252e-023	2.808e-023	-22.488	-22.552	-0.064
Fe(OH)4-2	4.946e-034	2.729e-034	-33.306	-33.564	-0.258
Fe(3)	8.549e-004				
Fe(OH)2+	5.591e-004	4.826e-004	-3.253	-3.316	-0.064
FeOH+2	2.685e-004	1.499e-004	-3.571	-3.824	-0.253
Fe+3	7.244e-006	2.389e-006	-5.140	-5.622	-0.482
Fe2(OH)2+4	5.711e-006	6.052e-007	-5.243	-6.218	-0.975
Fe(OH)3	2.194e-006	2.194e-006	-5.659	-5.659	0.000
Fe3(OH)4+5	1.905e-006	6.102e-008	-5.720	-7.215	-1.494
FeSO4+	7.807e-007	6.740e-007	-6.107	-6.171	-0.064
Fe(SO4)2-	3.848e-008	3.322e-008	-7.415	-7.479	-0.064
FeCO3+	2.746e-008	2.370e-008	-7.561	-7.625	-0.064
FeCl+2	6.128e-010	3.423e-010	-9.213	-9.466	-0.253

FeCl2+	2.760e-010	2.383e-010	-9.559	-9.623	-0.064
Fe(OH)4-	6.206e-012	5.357e-012	-11.207	-11.271	-0.064
FeCl4-	2.453e-019	2.117e-019	-18.610	-18.674	-0.064
H(0)	2.513e-033				
H2	1.256e-033	1.264e-033	-32.901	-32.898	0.002
K	9.258e-004				
K+	9.046e-004	7.759e-004	-3.044	-3.110	-0.067
KSO4-	2.115e-005	1.826e-005	-4.675	-4.739	-0.064
KCl	2.240e-008	2.240e-008	-7.650	-7.650	0.000
KHSO4	1.657e-009	1.657e-009	-8.781	-8.781	0.000
KOH	2.615e-014	2.615e-014	-13.583	-13.583	0.000
Mg	7.409e-004				
Mg+2	5.046e-004	3.032e-004	-3.297	-3.518	-0.221
MgSO4	2.360e-004	2.360e-004	-3.627	-3.627	0.000
MgCl+	2.357e-007	2.035e-007	-6.628	-6.691	-0.064
MgHCO3+	1.624e-008	1.402e-008	-7.789	-7.853	-0.064
MgCO3	5.509e-013	5.509e-013	-12.259	-12.259	0.000
Mg4(OH)4+4	1.266e-037	1.341e-038	-36.898	-37.873	-0.975
Mn(2)	1.895e-004				
Mn+2	1.337e-004	7.725e-005	-3.874	-4.112	-0.238
MnSO4	5.557e-005	5.557e-005	-4.255	-4.255	0.000
MnCl+	1.638e-007	1.414e-007	-6.786	-6.849	-0.064
MnHCO3+	2.713e-009	2.342e-009	-8.567	-8.630	-0.064
MnOH+	2.236e-011	1.930e-011	-10.651	-10.714	-0.064
MnCO3	4.645e-012	4.645e-012	-11.333	-11.333	0.000
MnCl3-	2.645e-014	2.284e-014	-13.578	-13.641	-0.064
Mn2OH+3	5.786e-015	1.598e-015	-14.238	-14.797	-0.559
Mn(OH)2	4.605e-019	4.605e-019	-18.337	-18.337	0.000
Mn2(OH)3+	7.992e-021	6.899e-021	-20.097	-20.161	-0.064
Mn(OH)3-	4.863e-027	4.199e-027	-26.313	-26.377	-0.064
Mn(OH)4-2	6.263e-037	3.456e-037	-36.203	-36.461	-0.258
Mn(3)	6.082e-019				
Mn+3	6.082e-019	1.679e-019	-18.216	-18.775	-0.559
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-46.754	-47.012	-0.258
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-45.392	-45.457	-0.065
Na	1.659e-003				
Na+	1.628e-003	1.405e-003	-2.788	-2.852	-0.064
NaSO4-	3.135e-005	2.707e-005	-4.504	-4.568	-0.064
NaCl	2.123e-007	2.123e-007	-6.673	-6.673	0.000
NaHCO3	8.004e-009	8.004e-009	-8.097	-8.097	0.000
NaOH	2.270e-014	2.270e-014	-13.644	-13.644	0.000
NaCO3-	9.782e-015	8.445e-015	-14.010	-14.073	-0.064
NaAlO2	1.975e-015	1.975e-015	-14.704	-14.704	0.000
O(0)	7.929e-027				
O2	3.964e-027	3.987e-027	-26.402	-26.399	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-88.985	-88.985	0.000
HS-	0.000e+000	0.000e+000	-91.942	-92.007	-0.065
S-2	0.000e+000	0.000e+000	-100.697	-100.945	-0.248
S2-2	0.000e+000	0.000e+000	-163.698	-163.956	-0.258
HAsS2	0.000e+000	0.000e+000	-187.368	-187.368	0.000
S3-2	0.000e+000	0.000e+000	-226.749	-227.008	-0.258
S4-2	0.000e+000	0.000e+000	-290.028	-290.287	-0.258
S5-2	0.000e+000	0.000e+000	-353.524	-353.782	-0.258
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-93.463	-93.721	-0.258
HS2O3-	0.000e+000	0.000e+000	-96.631	-96.695	-0.064
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-91.601	-91.849	-0.248
S(4)	2.297e-033				
HSO3-	2.261e-033	1.952e-033	-32.646	-32.710	-0.064
H2SO3	1.924e-035	1.924e-035	-34.716	-34.716	0.000
SO2	1.528e-035	1.528e-035	-34.816	-34.816	0.000
SO3-2	1.993e-036	1.113e-036	-35.700	-35.953	-0.253
S2O6-2	0.000e+000	0.000e+000	-50.957	-51.215	-0.258

S306-2	0.000e+000	0.000e+000	-116.491	-116.750	-0.258
S406-2	0.000e+000	0.000e+000	-166.121	-166.379	-0.258
S506-2	0.000e+000	0.000e+000	-244.629	-244.887	-0.258
S(5)	0.000e+000				
S205-2	0.000e+000	0.000e+000	-69.991	-70.249	-0.258
S(6)	6.948e-003				
SO4-2	5.284e-003	2.916e-003	-2.277	-2.535	-0.258
CaSO4	7.109e-004	7.109e-004	-3.148	-3.148	0.000
MgSO4	2.360e-004	2.360e-004	-3.627	-3.627	0.000
AlSO4+	2.199e-004	1.898e-004	-3.658	-3.722	-0.064
FeSO4	1.413e-004	1.413e-004	-3.850	-3.850	0.000
CuSO4	7.717e-005	7.717e-005	-4.113	-4.113	0.000
MnSO4	5.557e-005	5.557e-005	-4.255	-4.255	0.000
Al(SO4)2-	4.976e-005	4.296e-005	-4.303	-4.367	-0.064
ZnSO4	3.520e-005	3.520e-005	-4.453	-4.453	0.000
HSO4-	3.509e-005	3.029e-005	-4.455	-4.519	-0.064
NaSO4-	3.135e-005	2.707e-005	-4.504	-4.568	-0.064
KSO4-	2.115e-005	1.826e-005	-4.675	-4.739	-0.064
FeSO4+	7.807e-007	6.740e-007	-6.107	-6.171	-0.064
Fe(SO4)2-	3.848e-008	3.322e-008	-7.415	-7.479	-0.064
KHSO4	1.657e-009	1.657e-009	-8.781	-8.781	0.000
H2SO4	2.939e-012	2.939e-012	-11.532	-11.532	0.000
S(7)	0.000e+000				
S208-2	0.000e+000	0.000e+000	-48.443	-48.701	-0.258
S(8)	1.203e-037				
HSO5-	1.203e-037	1.039e-037	-36.920	-36.983	-0.064
Zn	1.348e-004				
Zn+2	9.946e-005	5.746e-005	-4.002	-4.241	-0.238
ZnSO4	3.520e-005	3.520e-005	-4.453	-4.453	0.000
ZnCl+	9.615e-008	8.300e-008	-7.017	-7.081	-0.064
ZnHCO3+	6.832e-009	5.898e-009	-8.165	-8.229	-0.064
ZnOH+	7.095e-010	6.125e-010	-9.149	-9.213	-0.064
ZnCl2	8.336e-011	8.336e-011	-10.079	-10.079	0.000
Zn(OH)Cl	1.379e-011	1.379e-011	-10.860	-10.860	0.000
ZnCO3	8.289e-013	8.289e-013	-12.082	-12.082	0.000
ZnCl3-	4.585e-014	3.958e-014	-13.339	-13.403	-0.064
Zn(OH)2	2.550e-014	2.550e-014	-13.593	-13.593	0.000
ZnCl4-2	4.675e-016	2.580e-016	-15.330	-15.588	-0.258
Zn(OH)3-	8.899e-022	7.682e-022	-21.051	-21.115	-0.064
Zn(OH)4-2	2.307e-030	1.273e-030	-29.637	-29.895	-0.258
ZnClO4+	0.000e+000	0.000e+000	-74.489	-74.553	-0.064

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

Phase	SI	log IAP	log KT	
Al	-122.35	27.57	149.91	Al
Al(g)	-173.05	27.57	200.62	Al
Al2(SO4)3	-34.90	-16.00	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-17.56	-16.00	1.56	Al2(SO4)3:6H2O
Alabandite	-91.71	-92.13	-0.42	MnS
Alum-K	-7.41	-12.38	-4.97	KAl(SO4)2:12H2O
Alunite	3.63	3.16	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.96	-5.31	-4.35	CaSO4
Antarcticite	-13.00	-8.91	4.09	CaCl2:6H2O
Antlerite	-7.13	1.60	8.73	Cu3(SO4)(OH)4
Aphthitalite	-13.37	-17.25	-3.89	NaK3(SO4)2
Aragonite	-6.16	-4.19	1.97	CaCO3
Arcanite	-6.91	-8.76	-1.84	K2SO4
Arsenolite	-31.88	-51.72	-19.84	As2O3
Arsenopyrite	-145.48	-159.93	-14.45	FeAsS
Artinite	-20.10	-0.47	19.63	Mg2CO3(OH)2:3H2O
As	-48.74	-6.06	42.68	As
As2O5	-19.19	-17.05	2.14	As2O5
As4O6(cubi)	-63.61	-103.44	-39.82	As4O6
As4O6(mono)	-63.39	-103.44	-40.05	As4O6
Atacamite	-12.22	2.05	14.26	Cu4Cl2(OH)6

Azurite	-15.78	-6.66	9.12	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$
Bassanite	-1.61	-5.31	-3.71	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
Birnessite	-60.10	-145.65	-85.55	$\text{Mn}_8\text{O}_{14} \cdot 5\text{H}_2\text{O}$
Bischofite	-14.04	-9.65	4.39	$\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$
Bixbyite	-12.66	-13.62	-0.96	$\text{Mn}_2\text{O}_3$
Bloedite	-11.82	-14.29	-2.48	$\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$
Boehmite	0.22	7.77	7.55	$\text{AlO}_2\text{H}$
Bornite	-305.44	-407.97	-102.53	$\text{Cu}_5\text{FeS}_4$
Brochantite	-9.78	5.64	15.42	$\text{Cu}_4(\text{SO}_4)(\text{OH})_6$
Brucite	-11.83	4.46	16.28	$\text{Mg}(\text{OH})_2$
Burkeite	-33.08	-23.60	9.49	$\text{Na}_6\text{CO}_3(\text{SO}_4)_2$
C	-47.13	17.01	64.15	C
C(g)	-164.75	17.01	181.77	C
Ca	-121.43	18.40	139.83	Ca
Ca(g)	-146.67	18.40	165.07	Ca
$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$	-33.64	25.93	59.57	$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$
$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$	-30.00	-3.71	26.29	$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$
$\text{Ca}_3(\text{AsO}_4)_2$	-19.26	-1.46	17.80	$\text{Ca}_3(\text{AsO}_4)_2$
$\text{Ca}_3\text{Al}_2\text{O}_6$	-81.90	31.13	113.03	$\text{Ca}_3\text{Al}_2\text{O}_6$
$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$	-91.47	49.01	140.48	$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$	-70.93	36.32	107.25	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$	-67.36	36.32	103.68	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$
$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$	-61.65	6.68	68.33	$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$
$\text{CaAl}_2\text{O}_4$	-26.18	20.73	46.91	$\text{CaAl}_2\text{O}_4$
$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$	-17.26	20.73	37.99	$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$
$\text{CaAl}_4\text{O}_7$	-32.33	36.27	68.59	$\text{CaAl}_4\text{O}_7$
Calcite	-6.01	-4.19	1.82	$\text{CaCO}_3$
Carnallite	-20.10	-15.83	4.27	$\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$
$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}(\text{beta})$	-1.78	-5.31	-3.54	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
$\text{CH}_4(\text{g})$	-97.84	-100.68	-2.84	$\text{CH}_4$
Chalcanthite	-3.84	-6.47	-2.63	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
Chalcocite	-77.50	-112.24	-34.74	$\text{Cu}_2\text{S}$
Chalcocyanite	-9.38	-6.47	2.91	$\text{CuSO}_4$
Chalcopyrite	-150.89	-183.49	-32.60	$\text{CuFeS}_2$
Chloromagnesite	-31.46	-9.65	21.82	$\text{MgCl}_2$
$\text{Cl}_2(\text{g})$	-30.30	-27.31	2.99	$\text{Cl}_2$
Claudetite	-31.92	-51.72	-19.80	$\text{As}_2\text{O}_3$
$\text{CO}(\text{g})$	-34.86	-37.86	-3.00	CO
$\text{CO}_2(\text{g})$	-1.56	-9.39	-7.83	$\text{CO}_2$
Corundum	-2.76	15.53	18.29	$\text{Al}_2\text{O}_3$
Covellite	-69.10	-91.96	-22.86	$\text{CuS}$
Cu	-14.26	17.24	31.50	Cu
$\text{Cu}(\text{g})$	-66.42	17.24	83.66	Cu
$\text{CuCl}_2$	-13.79	-10.07	3.72	$\text{CuCl}_2$
Cuprite	-14.34	-16.24	-1.91	$\text{Cu}_2\text{O}$
Dawsonite	-4.83	-0.49	4.34	$\text{NaAlCO}_3(\text{OH})_2$
Delafossite	4.66	-1.78	-6.44	$\text{CuFeO}_2$
Diaspore	0.62	7.77	7.15	$\text{AlHO}_2$
Dolomite	-11.59	-9.12	2.47	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-dis	-13.13	-9.12	4.01	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-ord	-11.58	-9.12	2.46	$\text{CaMg}(\text{CO}_3)_2$
Epsomite	-4.09	-6.05	-1.96	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$
Ettringite	-47.28	15.19	62.46	$\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O}$
Fe	-41.36	17.66	59.02	Fe
$\text{Fe}(\text{OH})_2$	-9.43	4.46	13.89	$\text{Fe}(\text{OH})_2$
$\text{Fe}(\text{OH})_3$	0.70	6.34	5.64	$\text{Fe}(\text{OH})_3$
$\text{Fe}_2(\text{SO}_4)_3$	-21.90	-18.85	3.05	$\text{Fe}_2(\text{SO}_4)_3$
FeO	-9.06	4.46	13.52	FeO
Ferrite-Ca	-3.61	17.88	21.50	$\text{CaFe}_2\text{O}_4$
Ferrite-Cu	6.44	16.72	10.28	$\text{CuFe}_2\text{O}_4$
Ferrite-Dicalcium	-33.72	23.08	56.80	$\text{Ca}_2\text{Fe}_2\text{O}_5$
Ferrite-Mg	-3.88	17.14	21.02	$\text{MgFe}_2\text{O}_4$
Ferrite-Zn	4.72	16.42	11.70	$\text{ZnFe}_2\text{O}_4$
$\text{FeSO}_4$	-8.66	-6.05	2.61	$\text{FeSO}_4$
Gaylussite	-22.47	-11.31	11.16	$\text{CaNa}_2(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$
Gibbsite	0.03	7.77	7.74	$\text{Al}(\text{OH})_3$
Glauberite	-8.08	-13.55	-5.47	$\text{Na}_2\text{Ca}(\text{SO}_4)_2$

Goethite	5.81	6.34	0.53	FeOOH
Gypsum	-0.78	-5.31	-4.53	CaSO4:2H2O
H2(g)	-29.80	-32.90	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-88.00	-95.99	-7.99	H2S
Halite	-7.48	-5.92	1.56	NaCl
Hausmannite	-19.90	-9.76	10.14	Mn3O4
HCl(g)	-13.36	-7.05	6.30	HCl
Hematite	12.61	12.68	0.08	Fe2O3
Hercynite	-8.81	19.99	28.80	FeAl2O4
Hexahydrite	-4.33	-6.05	-1.73	MgSO4:6H2O
Huntite	-29.20	-18.98	10.22	CaMg3(CO3)4
Hydromagnesite	-46.00	-15.27	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.65	-8.91	11.75	CaCl2
Hydrozincite	-30.41	-0.10	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	8.29	-1.12	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	4.59	-0.86	-5.45	NaFe3(SO4)2(OH)6
K	-63.50	7.48	70.98	K
K(g)	-74.10	7.48	81.58	K
K2CO3:1.5H2O	-21.01	-7.63	13.38	K2CO3:1.5H2O
K2O	-82.28	1.76	84.04	K2O
K3H(SO4)2	-14.77	-18.39	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-77.02	-49.31	27.71	K8H4(CO3)6:3H2O
Kainite	-11.92	-12.23	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.65	-12.38	3.27	KAl(SO4)2
Kalinite	-8.79	-8.51	0.28	KHCO3
Katoite	-47.82	31.13	78.94	Ca3Al2H12O12
Kieserite	-5.79	-6.05	-0.27	MgSO4:H2O
KMgCl3	-37.07	-15.83	21.25	KMgCl3
KMgCl3:2H2O	-29.79	-15.83	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-17.63	-7.38	10.26	KNaCO3:6H2O
Lammerite	-6.49	-4.94	1.55	Cu3(AsO4)2
Lansfordite	-9.77	-4.93	4.84	MgCO3:5H2O
Lawrencite	-18.70	-9.65	9.05	FeCl2
Leonite	-10.70	-14.81	-4.11	K2Mg(SO4)2:4H2O
Lime	-27.37	5.20	32.57	CaO
Magnesite	-7.20	-4.93	2.27	MgCO3
Magnetite	6.73	17.14	10.42	Fe3O4
Malachite	-7.21	-1.31	5.90	Cu2CO3(OH)2
Manganite	-6.65	-6.81	-0.16	MnO(OH)
Manganosite	-14.05	3.86	17.92	MnO
Mayenite	-323.04	171.11	494.15	Ca12Al14O33
Melanterite	-3.65	-6.05	-2.40	FeSO4:7H2O
Mercallite	-8.19	-9.63	-1.44	KHSO4
Mg	-104.86	17.66	122.52	Mg
Mg(g)	-124.59	17.66	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.13	-4.94	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-13.03	-3.83	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.38	-9.65	12.73	MgCl2:2H2O
MgCl2:4H2O	-16.95	-9.65	7.30	MgCl2:4H2O
MgCl2:H2O	-25.72	-9.65	16.07	MgCl2:H2O
MgOHCl	-18.49	-2.60	15.89	MgOHCl
MgSO4	-10.88	-6.05	4.83	MgSO4
Mirabilite	-7.09	-8.24	-1.15	Na2SO4:10H2O
Misenite	-55.48	-66.56	-11.08	K8H6(SO4)7
Mn	-65.87	17.06	82.93	Mn
Mn(OH)2(am)	-11.44	3.86	15.31	Mn(OH)2
Mn(OH)3	-13.15	-6.81	6.34	Mn(OH)3
MnCl2:2H2O	-14.24	-10.24	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.00	-10.24	2.75	MnCl2:4H2O
MnCl2:H2O	-15.79	-10.24	5.54	MnCl2:H2O
MnO2(gamma)	-9.44	-25.56	-16.13	MnO2
MnSO4	-9.26	-6.65	2.61	MnSO4
Molysite	-28.29	-14.82	13.47	FeCl3
Monohydrocalcite	-6.87	-4.19	2.68	CaCO3:H2O
Na	-59.64	7.74	67.37	Na

Na(g)	-73.12	7.74	80.86	Na
Na2CO3	-18.28	-7.12	11.16	Na2CO3
Na2CO3:7H2O	-17.06	-7.12	9.94	Na2CO3:7H2O
Na2O	-65.15	2.27	67.42	Na2O
Na3H(SO4)2	-16.72	-17.62	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-15.90	-21.79	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-12.41	7.48	19.88	NaFeO2
Nahcolite	-8.11	-8.25	-0.14	NaHCO3
Nantokite	-8.41	-15.18	-6.77	CuCl
Natron	-16.71	-7.12	9.59	Na2CO3:10H2O
Nesquehonite	-10.22	-4.93	5.29	MgCO3:3H2O
O2(g)	-23.51	-26.40	-2.89	O2
Orpiment	-260.22	-339.70	-79.49	As2S3
Oxychloride-Mg	-23.97	1.86	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.67	-6.05	-1.39	MgSO4:5H2O
Periclase	-16.87	4.46	21.33	MgO
Picromerite	-10.37	-14.81	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-22.63	-11.31	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-11.12	-25.44	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-17.35	5.20	22.55	Ca(OH)2
Pyrite	-141.46	-166.16	-24.70	FeS2
Pyrolusite	-7.90	-25.56	-17.66	MnO2
Pyrrhotite	-87.79	-91.53	-3.74	FeS
Realgar	-100.56	-160.84	-60.28	AsS
Rhodochrosite	-5.31	-5.52	-0.22	MnCO3
S	-64.08	-109.19	-45.11	S
S2(g)	-142.06	-149.25	-7.19	S2
Scacchite	-18.98	-10.24	8.74	MnCl2
Siderite	-4.71	-4.93	-0.22	FeCO3
Smithsonite	-6.10	-5.65	0.44	ZnCO3
SO2(g)	-34.99	-34.82	0.18	SO2
Sphalerite	-80.79	-92.26	-11.47	ZnS
Spinel	-17.61	19.99	37.61	Al2MgO4
Starkeyite	-5.05	-6.05	-1.00	MgSO4:4H2O
Sylvite	-7.00	-6.18	0.83	KCl
Syngenite	-6.47	-14.07	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.35	-28.21	17.14	Mg2CaCl6:12H2O
Tenorite	-3.61	4.04	7.65	CuO
Thenardite	-7.88	-8.24	-0.36	Na2SO4
Thermonatrite	-18.05	-7.12	10.94	Na2CO3:H2O
Todorokite	-50.03	-95.86	-45.82	Mn7O12:3H2O
Troilite	-87.69	-91.53	-3.84	FeS
Trona-K	-27.47	-15.88	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-83.09	-92.26	-9.17	ZnS
Wustite	-7.98	4.42	12.40	Fe.947O
Zincite	-7.46	3.73	11.20	ZnO
Zn	-51.85	16.93	68.79	Zn
Zn(ClO4)2:6H2O	-153.05	-147.42	5.63	Zn(ClO4)2:6H2O
Zn(g)	-68.47	16.93	85.41	Zn
Zn(OH)2(beta)	-8.20	3.73	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-7.93	3.73	11.66	Zn(OH)2
Zn(OH)2(gamma)	-8.15	3.73	11.88	Zn(OH)2
Zn2(OH)3Cl	-14.88	0.42	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-10.62	-3.04	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-15.16	-5.85	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-28.91	-9.82	19.09	Zn3O(SO4)2
ZnCl2	-17.45	-10.37	7.08	ZnCl2
ZnCO3:H2O	-5.79	-5.65	0.14	ZnCO3:H2O
ZnSO4	-10.31	-6.78	3.53	ZnSO4
ZnSO4:6H2O	-5.08	-6.78	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.90	-6.78	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.23	-6.78	-0.55	ZnSO4:H2O

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

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

-----  
End of run.  
-----