

Output file: C:\Users\usuairo\Dropbox (Taypi)\Taypi\03 PERSONAL\04 KATHERINA IBAÑEZ  
\archivos prheqc\listos\nuevos\finales\f2\mezcla25-75\MIX f2 \_1\_AS2\_3.pgo  
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat

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Reading data base.  
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LLNL\_AQUEOUS\_MODEL\_PARAMETERS  
NAMED\_EXPRESSIONS  
SOLUTION\_MASTER\_SPECIES  
SOLUTION\_SPECIES  
PHASES  
EXCHANGE\_MASTER\_SPECIES  
EXCHANGE\_SPECIES  
SURFACE\_MASTER\_SPECIES  
SURFACE\_SPECIES  
RATES  
END

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Reading input data for simulation 1.  
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DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat

SOLUTION 1 Flujo 2

temp	25
pH	2.80
pe	17
redox	pe
units	mg/l
density	1
Cl	45.3
S(6)	947.3
Al	8.4
As	0.3
Ca	34.9
Cu	0.1
Fe	43.4
K	15.8
Mg	11.5
Mn	6.0
Na	14.2
Zn	1.5
C(4)	0
water	1 # kg

SOLUTION 3 AS2

temp	25
units	mg/l
pe	10
pH	6.98
Cl	678.5
S(6)	427.00
Al	0.00
As	0.1526
Ca	238.3
Cu	0.00
Fe	0.00
K	40.73
Mg	13.69
Mn	0.114
Na	392.9
Zn	2.44
C(4)	153.72
MIX	2
1	1

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3      3
SELECTED_OUTPUT
file          DAM_AS2
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

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Beginning of initial solution calculations.  
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Initial solution 1.      Flujo 2

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

Elements	Molality	Moles
Al	3.117e-004	3.117e-004
As	4.009e-006	4.009e-006
Ca	8.718e-004	8.718e-004
Cl	1.279e-003	1.279e-003
Cu	1.575e-006	1.575e-006
Fe	7.780e-004	7.780e-004
K	4.046e-004	4.046e-004
Mg	4.737e-004	4.737e-004
Mn	1.093e-004	1.093e-004
Na	6.184e-004	6.184e-004
S(6)	9.875e-003	9.875e-003
Zn	2.297e-005	2.297e-005

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

```

pH = 2.800
pe = 17.000
Activity of water = 1.000
Ionic strength = 2.333e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -3.569e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.177e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -46.23
Iterations = 10
Total H = 1.110539e+002
Total O = 5.556546e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.790e-003	1.585e-003	-2.747	-2.800	-0.053
OH-	7.066e-012	6.077e-012	-11.151	-11.216	-0.065
H2O	5.553e+001	9.997e-001	1.744	-0.000	0.000
Al	3.117e-004				
AlSO4+	1.622e-004	1.400e-004	-3.790	-3.854	-0.064
Al+3	9.218e-005	3.030e-005	-4.035	-4.519	-0.483
Al(SO4)2-	5.687e-005	4.907e-005	-4.245	-4.309	-0.064
AlOH+2	3.842e-007	2.141e-007	-6.415	-6.669	-0.254
Al(OH)2+	3.635e-010	3.136e-010	-9.440	-9.504	-0.064
Al2(OH)2+4	7.091e-011	7.454e-012	-10.149	-11.128	-0.978
HALO2	2.880e-013	2.880e-013	-12.541	-12.541	0.000
Al3(OH)4+5	1.833e-015	5.800e-017	-14.737	-16.237	-1.500
AlO2-	7.214e-017	6.224e-017	-16.142	-16.206	-0.064
NaAlO2	6.150e-021	6.150e-021	-20.211	-20.211	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-64.935	-67.875	-2.940

As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-149.965	-149.965	0.000
As(3)	1.136e-026				
HAsO2	6.062e-027	6.062e-027	-26.217	-26.217	0.000
As(OH)3	5.299e-027	5.299e-027	-26.276	-26.276	0.000
H2AsO3-	2.370e-033	2.045e-033	-32.625	-32.689	-0.064
AsO2-	2.266e-033	1.955e-033	-32.645	-32.709	-0.064
AsO2OH-2	0.000e+000	0.000e+000	-40.640	-40.899	-0.259
As(5)	4.009e-006				
H2AsO4-	3.230e-006	2.787e-006	-5.491	-5.555	-0.064
H3AsO4	7.780e-007	7.780e-007	-6.109	-6.109	0.000
HAsO4-2	5.302e-010	2.919e-010	-9.276	-9.535	-0.259
AsO4-3	1.815e-018	4.725e-019	-17.741	-18.326	-0.584
Ca	8.718e-004				
Ca+2	6.315e-004	3.641e-004	-3.200	-3.439	-0.239
CaSO4	2.402e-004	2.402e-004	-3.619	-3.619	0.000
CaCl+	9.801e-008	8.456e-008	-7.009	-7.073	-0.064
CaCl2	1.090e-010	1.090e-010	-9.963	-9.963	0.000
CaOH+	3.760e-014	3.244e-014	-13.425	-13.489	-0.064
Cl(-1)	1.279e-003				
Cl-	1.278e-003	1.096e-003	-2.893	-2.960	-0.067
HCl	3.900e-007	3.900e-007	-6.409	-6.409	0.000
MgCl+	1.634e-007	1.410e-007	-6.787	-6.851	-0.064
MnCl+	1.037e-007	8.947e-008	-6.984	-7.048	-0.064
NaCl	9.975e-008	9.975e-008	-7.001	-7.001	0.000
CaCl+	9.801e-008	8.456e-008	-7.009	-7.073	-0.064
FeCl+2	2.048e-008	1.142e-008	-7.689	-7.942	-0.254
ZnCl+	1.825e-008	1.574e-008	-7.739	-7.803	-0.064
KCl	1.231e-008	1.231e-008	-7.910	-7.910	0.000
FeCl2+	1.174e-008	1.013e-008	-7.930	-7.995	-0.064
CuCl+	1.974e-009	1.703e-009	-8.705	-8.769	-0.064
CaCl2	1.090e-010	1.090e-010	-9.963	-9.963	0.000
ZnCl2	2.015e-011	2.015e-011	-10.696	-10.696	0.000
FeCl+	6.033e-012	5.206e-012	-11.219	-11.284	-0.064
CuCl2	9.828e-013	9.828e-013	-12.008	-12.008	0.000
Zn(OH)Cl	1.698e-013	1.698e-013	-12.770	-12.770	0.000
MnCl3-	2.720e-014	2.347e-014	-13.565	-13.630	-0.064
ZnCl3-	1.413e-014	1.219e-014	-13.850	-13.914	-0.064
ZnCl4-2	1.840e-016	1.013e-016	-15.735	-15.994	-0.259
FeCl2	3.061e-017	3.061e-017	-16.514	-16.514	0.000
FeCl4-	1.694e-017	1.462e-017	-16.771	-16.835	-0.064
CuCl2-	2.868e-022	2.474e-022	-21.542	-21.607	-0.064
FeCl4-2	1.929e-022	1.062e-022	-21.715	-21.974	-0.259
CuCl4-2	4.022e-023	2.214e-023	-22.396	-22.655	-0.259
CuCl3-2	3.163e-024	1.741e-024	-23.500	-23.759	-0.259
Cl(1)	1.997e-017				
HClO	1.997e-017	1.997e-017	-16.700	-16.700	0.000
ClO-	3.937e-022	3.397e-022	-21.405	-21.469	-0.064
Cl(3)	4.701e-033				
HClO2	3.145e-033	3.145e-033	-32.502	-32.502	0.000
ClO2-	1.556e-033	1.342e-033	-32.808	-32.872	-0.064
Cl(5)	4.389e-031				
ClO3-	4.389e-031	3.775e-031	-30.358	-30.423	-0.065
Cl(7)	6.162e-033				
ClO4-	6.161e-033	5.299e-033	-32.210	-32.276	-0.065
ZnClO4+	9.934e-037	8.571e-037	-36.003	-36.067	-0.064
Cu(1)	3.896e-021				
Cu+	3.606e-021	3.111e-021	-20.443	-20.507	-0.064
CuCl2-	2.868e-022	2.474e-022	-21.542	-21.607	-0.064
CuCl3-2	3.163e-024	1.741e-024	-23.500	-23.759	-0.259
Cu(2)	1.575e-006				
Cu+2	9.856e-007	5.683e-007	-6.006	-6.245	-0.239
CuSO4	5.878e-007	5.878e-007	-6.231	-6.231	0.000
CuCl+	1.974e-009	1.703e-009	-8.705	-8.769	-0.064
CuOH+	2.143e-011	1.849e-011	-10.669	-10.733	-0.064
CuCl2	9.828e-013	9.828e-013	-12.008	-12.008	0.000
CuCl4-2	4.022e-023	2.214e-023	-22.396	-22.655	-0.259

CuO2-2	5.806e-035	3.196e-035	-34.236	-34.495	-0.259
Fe(2)	1.598e-008				
Fe+2	1.131e-008	6.521e-009	-7.947	-8.186	-0.239
FeSO4	4.667e-009	4.667e-009	-8.331	-8.331	0.000
FeCl+	6.033e-012	5.206e-012	-11.219	-11.284	-0.064
FeOH+	1.508e-015	1.301e-015	-14.822	-14.886	-0.064
FeCl2	3.061e-017	3.061e-017	-16.514	-16.514	0.000
FeCl4-2	1.929e-022	1.062e-022	-21.715	-21.974	-0.259
Fe(OH)2	6.518e-024	6.518e-024	-23.186	-23.186	0.000
Fe(OH)3-	1.897e-031	1.637e-031	-30.722	-30.786	-0.064
Fe(OH)4-2	0.000e+000	0.000e+000	-42.727	-42.986	-0.259
Fe(3)	7.780e-004				
FeOH+2	4.569e-004	2.547e-004	-3.340	-3.594	-0.254
Fe+3	1.902e-004	6.253e-005	-3.721	-4.204	-0.483
Fe(OH)2+	6.165e-005	5.319e-005	-4.210	-4.274	-0.064
FeSO4+	3.166e-005	2.732e-005	-4.499	-4.564	-0.064
Fe2(OH)2+4	1.661e-005	1.745e-006	-4.780	-5.758	-0.978
Fe(SO4)2-	2.417e-006	2.085e-006	-5.617	-5.681	-0.064
Fe3(OH)4+5	6.129e-007	1.940e-008	-6.213	-7.712	-1.500
FeCl+2	2.048e-008	1.142e-008	-7.689	-7.942	-0.254
Fe(OH)3	1.569e-008	1.569e-008	-7.804	-7.804	0.000
FeCl2+	1.174e-008	1.013e-008	-7.930	-7.995	-0.064
Fe(OH)4-	2.882e-015	2.487e-015	-14.540	-14.604	-0.064
FeCl4-	1.694e-017	1.462e-017	-16.771	-16.835	-0.064
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-42.703	-42.700	0.002
K	4.046e-004				
K+	3.904e-004	3.346e-004	-3.408	-3.475	-0.067
KSO4-	1.414e-005	1.220e-005	-4.850	-4.914	-0.064
KHSO4	1.705e-008	1.705e-008	-7.768	-7.768	0.000
KCl	1.231e-008	1.231e-008	-7.910	-7.910	0.000
KOH	7.319e-016	7.319e-016	-15.136	-15.136	0.000
Mg	4.737e-004				
Mg+2	2.748e-004	1.648e-004	-3.561	-3.783	-0.222
MgSO4	1.987e-004	1.987e-004	-3.702	-3.702	0.000
MgCl+	1.634e-007	1.410e-007	-6.787	-6.851	-0.064
Mg4(OH)4+4	0.000e+000	0.000e+000	-42.704	-43.682	-0.978
Mn(2)	1.093e-004				
Mn+2	6.651e-005	3.835e-005	-4.177	-4.416	-0.239
MnSO4	4.272e-005	4.272e-005	-4.369	-4.369	0.000
MnCl+	1.037e-007	8.947e-008	-6.984	-7.048	-0.064
MnOH+	7.206e-013	6.218e-013	-12.142	-12.206	-0.064
MnCl3-	2.720e-014	2.347e-014	-13.565	-13.630	-0.064
Mn2OH+3	9.297e-017	2.555e-017	-16.032	-16.593	-0.561
Mn(OH)2	9.628e-022	9.628e-022	-21.016	-21.016	0.000
Mn2(OH)3+	5.386e-025	4.647e-025	-24.269	-24.333	-0.064
Mn(OH)3-	6.602e-031	5.696e-031	-30.180	-30.244	-0.064
Mn(OH)4-2	0.000e+000	0.000e+000	-41.257	-41.517	-0.259
Mn(3)	3.722e-013				
Mn+3	3.722e-013	1.023e-013	-12.429	-12.990	-0.561
Mn(6)	6.246e-033				
MnO4-2	6.246e-033	3.439e-033	-32.204	-32.464	-0.259
Mn(7)	1.761e-025				
MnO4-	1.761e-025	1.514e-025	-24.754	-24.820	-0.065
Na	6.184e-004				
Na+	6.004e-004	5.180e-004	-3.222	-3.286	-0.064
NaSO4-	1.791e-005	1.545e-005	-4.747	-4.811	-0.064
NaCl	9.975e-008	9.975e-008	-7.001	-7.001	0.000
NaOH	5.431e-016	5.431e-016	-15.265	-15.265	0.000
NaAlO2	6.150e-021	6.150e-021	-20.211	-20.211	0.000
O(0)	3.186e-007				
O2	1.593e-007	1.602e-007	-6.798	-6.795	0.002
S(6)	9.875e-003				
SO4-2	8.202e-003	4.515e-003	-2.086	-2.345	-0.259
HSO4-	8.378e-004	7.229e-004	-3.077	-3.141	-0.064
CaSO4	2.402e-004	2.402e-004	-3.619	-3.619	0.000
MgSO4	1.987e-004	1.987e-004	-3.702	-3.702	0.000

AlSO4+	1.622e-004	1.400e-004	-3.790	-3.854	-0.064
Al(SO4)2-	5.687e-005	4.907e-005	-4.245	-4.309	-0.064
MnSO4	4.272e-005	4.272e-005	-4.369	-4.369	0.000
FeSO4+	3.166e-005	2.732e-005	-4.499	-4.564	-0.064
NaSO4-	1.791e-005	1.545e-005	-4.747	-4.811	-0.064
KSO4-	1.414e-005	1.220e-005	-4.850	-4.914	-0.064
ZnSO4	8.114e-006	8.114e-006	-5.091	-5.091	0.000
Fe(SO4)2-	2.417e-006	2.085e-006	-5.617	-5.681	-0.064
CuSO4	5.878e-007	5.878e-007	-6.231	-6.231	0.000
KHSO4	1.705e-008	1.705e-008	-7.768	-7.768	0.000
FeSO4	4.667e-009	4.667e-009	-8.331	-8.331	0.000
H2SO4	1.081e-009	1.081e-009	-8.966	-8.966	0.000
Zn	2.297e-005				
Zn+2	1.483e-005	8.552e-006	-4.829	-5.068	-0.239
ZnSO4	8.114e-006	8.114e-006	-5.091	-5.091	0.000
ZnCl+	1.825e-008	1.574e-008	-7.739	-7.803	-0.064
ZnCl2	2.015e-011	2.015e-011	-10.696	-10.696	0.000
ZnOH+	6.857e-012	5.916e-012	-11.164	-11.228	-0.064
Zn(OH)Cl	1.698e-013	1.698e-013	-12.770	-12.770	0.000
ZnCl3-	1.413e-014	1.219e-014	-13.850	-13.914	-0.064
ZnCl4-2	1.840e-016	1.013e-016	-15.735	-15.994	-0.259
Zn(OH)2	1.598e-017	1.598e-017	-16.796	-16.796	0.000
Zn(OH)3-	3.622e-026	3.125e-026	-25.441	-25.505	-0.064
Zn(OH)4-2	6.104e-036	3.361e-036	-35.214	-35.474	-0.259
ZnClO4+	9.934e-037	8.571e-037	-36.003	-36.067	-0.064

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

Phase	SI	log IAP	log KT	
Al	-140.94	8.98	149.91	Al
Al(g)	-191.64	8.98	200.62	Al
Al2(SO4)3	-34.97	-16.07	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-17.63	-16.07	1.56	Al2(SO4)3:6H2O
Alum-K	-7.72	-12.69	-4.97	KAl(SO4)2:12H2O
Alunite	-4.45	-4.92	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.43	-5.78	-4.35	CaSO4
Antarcticite	-13.45	-9.36	4.09	CaCl2:6H2O
Antlerite	-18.61	-9.88	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.51	-18.40	-3.89	NaK3(SO4)2
Arcanite	-7.45	-9.30	-1.84	K2SO4
Arsenolite	-51.14	-70.98	-19.84	As2O3
As	-73.08	-30.39	42.68	As
As2O5	-18.84	-16.71	2.14	As2O5
As4O6(cubi)	-102.13	-141.96	-39.82	As4O6
As4O6(mono)	-101.91	-141.96	-40.05	As4O6
Atacamite	-28.37	-14.10	14.26	Cu4Cl2(OH)6
Bassanite	-2.08	-5.78	-3.71	CaSO4:0.5H2O
Birnessite	-22.73	-108.27	-85.55	Mn8O14:5H2O
Bischofite	-14.10	-9.70	4.39	MgCl2:6H2O
Bixbyite	-8.22	-9.18	-0.96	Mn2O3
Bloedite	-12.57	-15.05	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-3.67	3.88	7.55	AlO2H
Brochantite	-25.95	-10.53	15.42	Cu4(SO4)(OH)6
Brucite	-14.47	1.82	16.28	Mg(OH)2
Ca	-134.27	5.56	139.83	Ca
Ca(g)	-159.51	5.56	165.07	Ca
Ca2Al2O5:8H2O	-47.48	12.08	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-33.49	-7.20	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-28.03	-10.23	17.80	Ca3(AsO4)2
Ca3Al2O6	-98.79	14.25	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-115.68	24.80	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-90.85	16.41	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-87.28	16.40	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-71.21	-2.88	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-36.98	9.92	46.91	CaAl2O4
CaAl2O4:10H2O	-28.07	9.92	37.99	CaAl2O4:10H2O

CaAl4O7	-50.90	17.69	68.59	CaAl4O7
Carnallite	-20.41	-16.14	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.25	-5.78	-3.54	CaSO4:0.5H2O
Chalcanthite	-5.96	-8.59	-2.63	CuSO4:5H2O
Chalcocyanite	-11.50	-8.59	2.91	CuSO4
Chloromagnesite	-31.52	-9.70	21.82	MgCl2
Cl2(g)	-17.91	-14.92	2.99	Cl2
Claudetite	-51.18	-70.98	-19.80	As2O3
Corundum	-10.53	7.76	18.29	Al2O3
Cu	-28.74	2.75	31.50	Cu
Cu(g)	-80.90	2.75	83.66	Cu
CuCl2	-15.89	-12.17	3.72	CuCl2
Cuprite	-33.51	-35.41	-1.91	Cu2O
Delafoosite	-7.08	-13.51	-6.44	CuFeO2
Diaspore	-3.27	3.88	7.15	AlHO2
Epsomite	-4.17	-6.13	-1.96	MgSO4:7H2O
Ettringite	-65.57	-3.11	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-58.21	0.81	59.02	Fe
Fe(OH)2	-16.48	-2.59	13.89	Fe(OH)2
Fe(OH)3	-1.44	4.20	5.64	Fe(OH)3
Fe2(SO4)3	-18.49	-15.44	3.05	Fe2(SO4)3
FeO	-16.11	-2.59	13.52	FeO
Ferrite-Ca	-10.94	10.55	21.50	CaFe2O4
Ferrite-Cu	-2.54	7.75	10.28	CuFe2O4
Ferrite-Dicalcium	-44.08	12.71	56.80	Ca2Fe2O5
Ferrite-Mg	-10.81	10.21	21.02	MgFe2O4
Ferrite-Zn	-2.78	8.92	11.70	ZnFe2O4
FeSO4	-13.14	-10.53	2.61	FeSO4
Gibbsite	-3.86	3.88	7.74	Al(OH)3
Glauberite	-9.23	-14.70	-5.47	Na2Ca(SO4)2
Goethite	3.67	4.20	0.53	FeOOH
Gypsum	-1.25	-5.78	-4.53	CaSO4:2H2O
H2(g)	-39.60	-42.70	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.81	-6.25	1.56	NaCl
Hausmannite	-18.14	-8.00	10.14	Mn3O4
HCl(g)	-12.06	-5.76	6.30	HCl
Hematite	8.32	8.39	0.08	Fe2O3
Hercynite	-23.63	5.18	28.80	FeAl2O4
Hexahydrite	-4.40	-6.13	-1.73	MgSO4:6H2O
Hydrophilite	-21.11	-9.36	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	5.43	-3.98	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	1.66	-3.79	-5.45	NaFe3(SO4)2(OH)6
K	-69.95	1.02	70.98	K
K(g)	-80.56	1.02	81.58	K
K2O	-85.39	-1.35	84.04	K2O
K3H(SO4)2	-14.29	-17.92	-3.62	K3H(SO4)2
Kainite	-12.25	-12.56	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.96	-12.68	3.27	KAl(SO4)2
Katoite	-64.70	14.25	78.94	Ca3Al2H12O12
Kieserite	-5.86	-6.13	-0.27	MgSO4:H2O
KMgCl3	-37.39	-16.14	21.25	KMgCl3
KMgCl3:2H2O	-30.10	-16.14	13.96	KMgCl3:2H2O
Lammerite	-20.20	-18.65	1.55	Cu3(AsO4)2
Lawrencite	-23.16	-14.11	9.05	FeCl2
Leonite	-11.31	-15.42	-4.11	K2Mg(SO4)2:4H2O
Lime	-30.41	2.16	32.57	CaO
Magnetite	-4.61	5.81	10.42	Fe3O4
Manganite	-4.43	-4.59	-0.16	MnO(OH)
Manganosite	-16.73	1.18	17.92	MnO
Mayenite	-413.88	80.27	494.15	Ca12Al14O33
Melanterite	-8.13	-10.53	-2.40	FeSO4:7H2O
Mercallite	-7.18	-8.62	-1.44	KHSO4
Mg	-117.31	5.21	122.52	Mg
Mg(g)	-137.03	5.21	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.87	-5.67	5.20	Mg1.25SO4(OH)0.5:0.5H2O

Mg1.5SO4(OH)	-14.43	-5.22	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.44	-9.70	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.01	-9.70	7.30	MgCl2:4H2O
MgCl2:H2O	-25.78	-9.70	16.07	MgCl2:H2O
MgOHCl	-19.83	-3.94	15.89	MgOHCl
MgSO4	-10.96	-6.13	4.83	MgSO4
Mirabilite	-7.76	-8.92	-1.15	Na2SO4:10H2O
Misenite	-49.94	-61.02	-11.08	K8H6(SO4)7
Mn	-78.35	4.58	82.93	Mn
Mn(OH)2(am)	-14.12	1.18	15.31	Mn(OH)2
Mn(OH)3	-10.93	-4.59	6.34	Mn(OH)3
MnCl2:2H2O	-14.33	-10.34	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.09	-10.34	2.75	MnCl2:4H2O
MnCl2:H2O	-15.88	-10.34	5.54	MnCl2:H2O
MnO2(gamma)	-2.31	-18.44	-16.13	MnO2
MnSO4	-9.37	-6.76	2.61	MnSO4
Molysite	-26.56	-13.08	13.47	FeCl3
Na	-66.16	1.21	67.37	Na
Na(g)	-79.65	1.21	80.86	Na
Na2O	-68.39	-0.97	67.42	Na2O
Na3H(SO4)2	-16.46	-17.35	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-17.72	-23.62	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-16.17	3.71	19.88	NaFeO2
Nantokite	-16.70	-23.47	-6.77	CuCl
O2(g)	-3.90	-6.80	-2.89	O2
Oxychloride-Mg	-27.96	-2.13	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.74	-6.13	-1.39	MgSO4:5H2O
Periclase	-19.51	1.82	21.33	MgO
Picromerite	-10.99	-15.43	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-12.68	-26.99	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-20.39	2.16	22.55	Ca(OH)2
Pyrolusite	-0.78	-18.44	-17.66	MnO2
Scacchite	-19.08	-10.34	8.74	MnCl2
Spinel	-28.03	9.58	37.61	Al2MgO4
Starkeyite	-5.13	-6.13	-1.00	MgSO4:4H2O
Sylvite	-7.26	-6.44	0.83	KCl
Syngenite	-7.48	-15.08	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-45.91	-28.77	17.14	Mg2CaCl6:12H2O
Tenorite	-8.29	-0.65	7.65	CuO
Thenardite	-8.56	-8.92	-0.36	Na2SO4
Todorokite	-19.78	-65.61	-45.82	Mn7O12:3H2O
Wustite	-14.13	-1.73	12.40	Fe.9470
Zincite	-10.67	0.53	11.20	ZnO
Zn	-64.86	3.93	68.79	Zn
Zn(ClO4)2:6H2O	-75.25	-69.62	5.63	Zn(ClO4)2:6H2O
Zn(g)	-81.48	3.93	85.41	Zn
Zn(OH)2(beta)	-11.40	0.53	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-11.13	0.53	11.66	Zn(OH)2
Zn(OH)2(gamma)	-11.35	0.53	11.88	Zn(OH)2
Zn2(OH)3Cl	-19.99	-4.70	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-14.46	-6.88	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-24.43	-15.11	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-33.38	-14.29	19.09	Zn3O(SO4)2
ZnCl2	-18.07	-10.99	7.08	ZnCl2
ZnSO4	-10.95	-7.41	3.53	ZnSO4
ZnSO4:6H2O	-5.71	-7.41	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.54	-7.41	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.86	-7.41	-0.55	ZnSO4:H2O

Initial solution 3. AS2

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

Elements	Molality	Moles
As	2.041e-006	2.041e-006
C(4)	2.525e-003	2.525e-003

Ca	5.958e-003	5.958e-003
Cl	1.918e-002	1.918e-002
K	1.044e-003	1.044e-003
Mg	5.644e-004	5.644e-004
Mn	2.079e-006	2.079e-006
Na	1.712e-002	1.712e-002
S(6)	4.455e-003	4.455e-003
Zn	3.739e-005	3.739e-005

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

pH	=	6.980
pe	=	10.000
Activity of water	=	0.999
Ionic strength	=	3.800e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.128e-003
Total CO2 (mol/kg)	=	2.525e-003
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	1.075e-003
Percent error, 100*(Cat- An )/(Cat+ An )	=	1.86
Iterations	=	4
Total H	=	1.110528e+002
Total O	=	5.555032e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.207e-007	1.047e-007	-6.918	-6.980	-0.062
OH-	1.105e-007	9.193e-008	-6.957	-7.037	-0.080
H2O	5.553e+001	9.992e-001	1.744	-0.000	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-132.370	-132.370	0.000
As(3)	5.398e-026				
HAsO2	2.863e-026	2.863e-026	-25.543	-25.543	0.000
As(OH)3	2.501e-026	2.501e-026	-25.602	-25.602	0.000
H2AsO3-	1.747e-028	1.461e-028	-27.758	-27.835	-0.078
AsO2-	1.672e-028	1.398e-028	-27.777	-27.855	-0.078
AsO2OH-2	2.820e-032	1.363e-032	-31.550	-31.866	-0.316
As(5)	2.041e-006				
HAsO4-2	1.495e-006	7.226e-007	-5.825	-6.141	-0.316
H2AsO4-	5.453e-007	4.559e-007	-6.263	-6.341	-0.078
AsO4-3	9.134e-011	1.770e-011	-10.039	-10.752	-0.713
H3AsO4	8.408e-012	8.408e-012	-11.075	-11.075	0.000
C(4)	2.525e-003				
HCO3-	2.009e-003	1.680e-003	-2.697	-2.775	-0.078
CO2	4.046e-004	4.084e-004	-3.393	-3.389	0.004
CaHCO3+	6.422e-005	5.369e-005	-4.192	-4.270	-0.078
NaHCO3	3.387e-005	3.387e-005	-4.470	-4.470	0.000
MgHCO3+	5.687e-006	4.755e-006	-5.245	-5.323	-0.078
CaCO3	4.449e-006	4.449e-006	-5.352	-5.352	0.000
CO3-2	1.446e-006	7.117e-007	-5.840	-6.148	-0.308
ZnHCO3+	8.088e-007	6.762e-007	-6.092	-6.170	-0.078
MgCO3	1.835e-007	1.835e-007	-6.736	-6.736	0.000
ZnCO3	9.333e-008	9.333e-008	-7.030	-7.030	0.000
NaCO3-	4.199e-008	3.511e-008	-7.377	-7.455	-0.078
MnCO3	2.132e-008	2.132e-008	-7.671	-7.671	0.000
MnHCO3+	1.309e-008	1.095e-008	-7.883	-7.961	-0.078
Ca	5.958e-003				
Ca+2	5.216e-003	2.697e-003	-2.283	-2.569	-0.286
CaSO4	6.619e-004	6.619e-004	-3.179	-3.179	0.000
CaHCO3+	6.422e-005	5.369e-005	-4.192	-4.270	-0.078
CaCl+	1.082e-005	9.048e-006	-4.966	-5.043	-0.078
CaCO3	4.449e-006	4.449e-006	-5.352	-5.352	0.000
CaCl2	1.685e-007	1.685e-007	-6.774	-6.774	0.000

CaOH+	4.348e-009	3.635e-009	-8.362	-8.439	-0.078
Cl(-1)	1.918e-002				
Cl-	1.912e-002	1.583e-002	-1.719	-1.801	-0.082
NaCl	3.922e-005	3.922e-005	-4.407	-4.407	0.000
CaCl+	1.082e-005	9.048e-006	-4.966	-5.043	-0.078
MgCl+	3.602e-006	3.011e-006	-5.443	-5.521	-0.078
ZnCl+	4.967e-007	4.153e-007	-6.304	-6.382	-0.078
KCl	4.530e-007	4.530e-007	-6.344	-6.344	0.000
CaCl2	1.685e-007	1.685e-007	-6.774	-6.774	0.000
Zn(OH)Cl	6.775e-008	6.775e-008	-7.169	-7.169	0.000
MnCl+	3.450e-008	2.885e-008	-7.462	-7.540	-0.078
ZnCl2	7.678e-009	7.678e-009	-8.115	-8.115	0.000
HCl	3.723e-010	3.723e-010	-9.429	-9.429	0.000
ZnCl3-	8.028e-011	6.712e-011	-10.095	-10.173	-0.078
ZnCl4-2	1.666e-011	8.053e-012	-10.778	-11.094	-0.316
MnCl3-	1.888e-012	1.579e-012	-11.724	-11.802	-0.078
Cl(1)	5.707e-026				
HClO	4.363e-026	4.363e-026	-25.360	-25.360	0.000
ClO-	1.344e-026	1.124e-026	-25.872	-25.949	-0.078
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-42.915	-42.993	-0.078
HClO2	0.000e+000	0.000e+000	-46.803	-46.803	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-46.104	-46.184	-0.080
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-53.597	-53.677	-0.080
ZnClO4+	0.000e+000	0.000e+000	-57.129	-57.207	-0.078
H(0)	1.724e-037				
H2	8.621e-038	8.701e-038	-37.064	-37.060	0.004
K	1.044e-003				
K+	1.029e-003	8.522e-004	-2.987	-3.069	-0.082
KSO4-	1.382e-005	1.156e-005	-4.859	-4.937	-0.078
KCl	4.530e-007	4.530e-007	-6.344	-6.344	0.000
KOH	2.820e-011	2.820e-011	-10.550	-10.550	0.000
KHSO4	1.068e-012	1.068e-012	-11.972	-11.972	0.000
Mg	5.644e-004				
Mg+2	4.456e-004	2.437e-004	-3.351	-3.613	-0.262
MgSO4	1.093e-004	1.093e-004	-3.961	-3.961	0.000
MgHCO3+	5.687e-006	4.755e-006	-5.245	-5.323	-0.078
MgCl+	3.602e-006	3.011e-006	-5.443	-5.521	-0.078
MgCO3	1.835e-007	1.835e-007	-6.736	-6.736	0.000
Mg4(OH)4+4	7.829e-026	5.199e-027	-25.106	-26.284	-1.178
Mn(2)	2.079e-006				
Mn+2	1.655e-006	8.558e-007	-5.781	-6.068	-0.286
MnSO4	3.548e-007	3.548e-007	-6.450	-6.450	0.000
MnCl+	3.450e-008	2.885e-008	-7.462	-7.540	-0.078
MnCO3	2.132e-008	2.132e-008	-7.671	-7.671	0.000
MnHCO3+	1.309e-008	1.095e-008	-7.883	-7.961	-0.078
MnOH+	2.511e-010	2.099e-010	-9.600	-9.678	-0.078
MnCl3-	1.888e-012	1.579e-012	-11.724	-11.802	-0.078
Mn(OH)2	4.917e-015	4.917e-015	-14.308	-14.308	0.000
Mn2(OH)3+	9.583e-016	8.011e-016	-15.019	-15.096	-0.078
Mn2OH+3	9.169e-016	1.925e-016	-15.038	-15.716	-0.678
Mn(OH)3-	5.264e-020	4.400e-020	-19.279	-19.357	-0.078
Mn(OH)4-2	7.358e-027	3.556e-027	-26.133	-26.449	-0.316
Mn(3)	1.087e-021				
Mn+3	1.087e-021	2.283e-022	-20.964	-21.642	-0.678
Mn(6)	4.364e-029				
MnO4-2	4.364e-029	2.109e-029	-28.360	-28.676	-0.316
Mn(7)	1.116e-028				
MnO4-	1.116e-028	9.286e-029	-27.952	-28.032	-0.080
Na	1.712e-002				
Na+	1.686e-002	1.410e-002	-1.773	-1.851	-0.078
NaSO4-	1.872e-004	1.565e-004	-3.728	-3.806	-0.078
NaCl	3.922e-005	3.922e-005	-4.407	-4.407	0.000
NaHCO3	3.387e-005	3.387e-005	-4.470	-4.470	0.000
NaCO3-	4.199e-008	3.511e-008	-7.377	-7.455	-0.078

NaOH	2.236e-010	2.236e-010	-9.651	-9.651	0.000
O(0)	1.664e-018				
O2	8.321e-019	8.398e-019	-18.080	-18.076	0.004
S(6)	4.455e-003				
SO4-2	3.477e-003	1.680e-003	-2.459	-2.775	-0.316
CaSO4	6.619e-004	6.619e-004	-3.179	-3.179	0.000
NaSO4-	1.872e-004	1.565e-004	-3.728	-3.806	-0.078
MgSO4	1.093e-004	1.093e-004	-3.961	-3.961	0.000
KSO4-	1.382e-005	1.156e-005	-4.859	-4.937	-0.078
ZnSO4	5.512e-006	5.512e-006	-5.259	-5.259	0.000
MnSO4	3.548e-007	3.548e-007	-6.450	-6.450	0.000
HSO4-	2.126e-008	1.777e-008	-7.673	-7.750	-0.078
KHSO4	1.068e-012	1.068e-012	-11.972	-11.972	0.000
H2SO4	1.756e-018	1.756e-018	-17.756	-17.756	0.000
Zn	3.739e-005				
Zn+2	3.020e-005	1.561e-005	-4.520	-4.806	-0.286
ZnSO4	5.512e-006	5.512e-006	-5.259	-5.259	0.000
ZnHCO3+	8.088e-007	6.762e-007	-6.092	-6.170	-0.078
ZnCl+	4.967e-007	4.153e-007	-6.304	-6.382	-0.078
ZnOH+	1.955e-007	1.634e-007	-6.709	-6.787	-0.078
ZnCO3	9.333e-008	9.333e-008	-7.030	-7.030	0.000
Zn(OH)Cl	6.775e-008	6.775e-008	-7.169	-7.169	0.000
ZnCl2	7.678e-009	7.678e-009	-8.115	-8.115	0.000
Zn(OH)2	6.677e-009	6.677e-009	-8.175	-8.175	0.000
ZnCl3-	8.028e-011	6.712e-011	-10.095	-10.173	-0.078
ZnCl4-2	1.666e-011	8.053e-012	-10.778	-11.094	-0.316
Zn(OH)3-	2.362e-013	1.975e-013	-12.627	-12.704	-0.078
Zn(OH)4-2	6.648e-019	3.213e-019	-18.177	-18.493	-0.316
ZnClO4+	0.000e+000	0.000e+000	-57.129	-57.207	-0.078

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

Phase	SI	log IAP	log KT	
Anhydrite	-0.99	-5.34	-4.35	CaSO4
Antarcticite	-10.27	-6.17	4.09	CaCl2:6H2O
Aphthitalite	-12.72	-16.61	-3.89	NaK3(SO4)2
Aragonite	-0.33	1.64	1.97	CaCO3
Arcanite	-7.07	-8.91	-1.84	K2SO4
Arsenolite	-49.79	-69.63	-19.84	As2O3
Artinite	-8.69	10.94	19.63	Mg2CO3(OH)2:3H2O
As	-63.94	-21.26	42.68	As
As2O5	-28.78	-26.64	2.14	As2O5
As4O6(cubi)	-99.44	-139.26	-39.82	As4O6
As4O6(mono)	-99.21	-139.26	-40.05	As4O6
Bassanite	-1.64	-5.34	-3.71	CaSO4:0.5H2O
Birnessite	-2.90	-88.45	-85.55	Mn8O14:5H2O
Bischofite	-11.61	-7.22	4.39	MgCl2:6H2O
Bixbyite	-0.44	-1.40	-0.96	Mn2O3
Bloedite	-10.39	-12.87	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-5.94	10.35	16.28	Mg(OH)2
Burkeite	-21.94	-12.45	9.49	Na6CO3(SO4)2
C	-55.82	8.32	64.15	C
C(g)	-173.44	8.32	181.77	C
Ca	-119.40	20.43	139.83	Ca
Ca(g)	-144.64	20.43	165.07	Ca
Ca2Cl2(OH)2:H2O	-21.07	5.22	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-10.27	7.53	17.80	Ca3(AsO4)2
Ca4Cl2(OH)6:13H2O	-40.33	28.00	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-0.19	1.64	1.82	CaCO3
Carnallite	-16.36	-12.09	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.81	-5.34	-3.54	CaSO4:0.5H2O
Chloromagnesite	-29.03	-7.21	21.82	MgCl2
Cl2(g)	-29.59	-26.60	2.99	Cl2
Claudetite	-49.83	-69.63	-19.80	As2O3
CO2(g)	-1.93	-9.75	-7.83	CO2
Dolomite	-0.25	2.23	2.47	CaMg(CO3)2

Dolomite-dis	-1.78	2.23	4.01	CaMg(CO <sub>3</sub> ) <sub>2</sub>
Dolomite-ord	-0.24	2.23	2.46	CaMg(CO <sub>3</sub> ) <sub>2</sub>
Epsomite	-4.43	-6.39	-1.96	MgSO <sub>4</sub> :7H <sub>2</sub> O
Gaylussite	-9.03	2.14	11.16	CaNa <sub>2</sub> (CO <sub>3</sub> ) <sub>2</sub> :5H <sub>2</sub> O
Glauberite	-6.35	-11.82	-5.47	Na <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub>
Gypsum	-0.81	-5.34	-4.53	CaSO <sub>4</sub> :2H <sub>2</sub> O
H <sub>2</sub> (g)	-33.96	-37.06	-3.10	H <sub>2</sub>
H <sub>2</sub> O(g)	-1.59	-0.00	1.59	H <sub>2</sub> O
Halite	-5.21	-3.65	1.56	NaCl
Hausmannite	-3.66	6.49	10.14	Mn <sub>3</sub> O <sub>4</sub>
HCl(g)	-15.08	-8.78	6.30	HCl
Hexahydrate	-4.66	-6.39	-1.73	MgSO <sub>4</sub> :6H <sub>2</sub> O
Huntite	-6.81	3.41	10.22	CaMg <sub>3</sub> (CO <sub>3</sub> ) <sub>4</sub>
Hydromagnesite	-18.03	12.71	30.74	Mg <sub>5</sub> (CO <sub>3</sub> ) <sub>4</sub> (OH) <sub>2</sub> :4H <sub>2</sub> O
Hydrophilite	-17.92	-6.17	11.75	CaCl <sub>2</sub>
Hydrozincite	-4.05	26.26	30.31	Zn <sub>5</sub> (OH) <sub>6</sub> (CO <sub>3</sub> ) <sub>2</sub>
Ice	-0.14	-0.00	0.14	H <sub>2</sub> O
K	-62.55	8.43	70.98	K
K(g)	-73.15	8.43	81.58	K
K <sub>2</sub> CO <sub>3</sub> :1.5H <sub>2</sub> O	-15.31	-1.93	13.38	K <sub>2</sub> CO <sub>3</sub> :1.5H <sub>2</sub> O
K <sub>2</sub> O	-76.21	7.82	84.04	K <sub>2</sub> O
K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>	-18.11	-21.74	-3.62	K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>
K <sub>8</sub> H <sub>4</sub> (CO <sub>3</sub> ) <sub>6</sub> :3H <sub>2</sub> O	-54.95	-27.24	27.71	K <sub>8</sub> H <sub>4</sub> (CO <sub>3</sub> ) <sub>6</sub> :3H <sub>2</sub> O
Kainite	-10.95	-11.26	-0.31	KMgClSO <sub>4</sub> :3H <sub>2</sub> O
Kaliginite	-6.13	-5.84	0.28	KHCO <sub>3</sub>
Kieserite	-6.12	-6.39	-0.27	MgSO <sub>4</sub> :H <sub>2</sub> O
KMgCl <sub>3</sub>	-33.33	-12.08	21.25	KMgCl <sub>3</sub>
KMgCl <sub>3</sub> :2H <sub>2</sub> O	-26.05	-12.08	13.96	KMgCl <sub>3</sub> :2H <sub>2</sub> O
KNaCO <sub>3</sub> :6H <sub>2</sub> O	-10.98	-0.72	10.26	KNaCO <sub>3</sub> :6H <sub>2</sub> O
Lansfordite	-4.25	0.59	4.84	MgCO <sub>3</sub> :5H <sub>2</sub> O
Leonite	-11.19	-15.30	-4.11	K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> :4H <sub>2</sub> O
Lime	-21.18	11.39	32.57	CaO
Magnesite	-1.68	0.59	2.27	MgCO <sub>3</sub>
Manganite	-0.54	-0.70	-0.16	MnO(OH)
Manganosite	-10.02	7.89	17.92	MnO
Mercallite	-11.39	-12.82	-1.44	KHSO <sub>4</sub>
Mg	-103.14	19.38	122.52	Mg
Mg(g)	-122.86	19.38	142.25	Mg
Mg <sub>1.25</sub> SO <sub>4</sub> (OH) <sub>0.5</sub> :0.5H <sub>2</sub> O	-9.00	-3.80	5.20	Mg <sub>1.25</sub> SO <sub>4</sub> (OH) <sub>0.5</sub> :0.5H <sub>2</sub> O
Mg <sub>1.5</sub> SO <sub>4</sub> (OH)	-10.42	-1.21	9.21	Mg <sub>1.5</sub> SO <sub>4</sub> (OH)
MgCl <sub>2</sub> :2H <sub>2</sub> O	-19.95	-7.21	12.73	MgCl <sub>2</sub> :2H <sub>2</sub> O
MgCl <sub>2</sub> :4H <sub>2</sub> O	-14.52	-7.22	7.30	MgCl <sub>2</sub> :4H <sub>2</sub> O
MgCl <sub>2</sub> :H <sub>2</sub> O	-23.29	-7.21	16.07	MgCl <sub>2</sub> :H <sub>2</sub> O
MgOHCl	-14.33	1.57	15.89	MgOHCl
MgSO <sub>4</sub>	-11.22	-6.39	4.83	MgSO <sub>4</sub>
Mirabilite	-5.33	-6.48	-1.15	Na <sub>2</sub> SO <sub>4</sub> :10H <sub>2</sub> O
Misenite	-74.78	-85.86	-11.08	K <sub>8</sub> H <sub>6</sub> (SO <sub>4</sub> ) <sub>7</sub>
Mn	-66.00	16.93	82.93	Mn
Mn(OH) <sub>2</sub> (am)	-7.42	7.89	15.31	Mn(OH) <sub>2</sub>
Mn(OH) <sub>3</sub>	-7.04	-0.70	6.34	Mn(OH) <sub>3</sub>
MnCl <sub>2</sub> :2H <sub>2</sub> O	-13.67	-9.67	4.00	MnCl <sub>2</sub> :2H <sub>2</sub> O
MnCl <sub>2</sub> :4H <sub>2</sub> O	-12.42	-9.67	2.75	MnCl <sub>2</sub> :4H <sub>2</sub> O
MnCl <sub>2</sub> :H <sub>2</sub> O	-15.21	-9.67	5.54	MnCl <sub>2</sub> :H <sub>2</sub> O
MnO <sub>2</sub> (gamma)	-1.25	-17.37	-16.13	MnO <sub>2</sub>
MnSO <sub>4</sub>	-11.45	-8.84	2.61	MnSO <sub>4</sub>
Monohydrocalcite	-1.04	1.64	2.68	CaCO <sub>3</sub> :H <sub>2</sub> O
Na	-57.72	9.65	67.37	Na
Na(g)	-71.21	9.65	80.86	Na
Na <sub>2</sub> CO <sub>3</sub>	-10.66	0.50	11.16	Na <sub>2</sub> CO <sub>3</sub>
Na <sub>2</sub> CO <sub>3</sub> :7H <sub>2</sub> O	-9.44	0.50	9.94	Na <sub>2</sub> CO <sub>3</sub> :7H <sub>2</sub> O
Na <sub>2</sub> O	-57.16	10.26	67.42	Na <sub>2</sub> O
Na <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>	-17.19	-18.08	-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	-12.40	-18.30	-5.89	Na <sub>4</sub> Ca(SO <sub>4</sub> ) <sub>3</sub> :2H <sub>2</sub> O
Nahcolite	-4.48	-4.63	-0.14	NaHCO <sub>3</sub>
Natron	-9.09	0.50	9.59	Na <sub>2</sub> CO <sub>3</sub> :10H <sub>2</sub> O
Nesquehonite	-4.70	0.59	5.29	MgCO <sub>3</sub> :3H <sub>2</sub> O
O <sub>2</sub> (g)	-15.18	-18.08	-2.89	O <sub>2</sub>

Oxychloride-Mg	-13.92	11.91	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-5.00	-6.39	-1.39	MgSO4:5H2O
Periclase	-10.98	10.35	21.33	MgO
Picromerite	-10.86	-15.30	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-9.18	2.14	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-11.68	-25.99	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-11.16	11.39	22.55	Ca(OH)2
Pyrolusite	0.29	-17.37	-17.66	MnO2
Rhodochrosite	-1.64	-1.86	-0.22	MnCO3
Scacchite	-18.41	-9.67	8.74	MnCl2
Smithsonite	-1.05	-0.60	0.44	ZnCO3
Starkeyite	-5.39	-6.39	-1.00	MgSO4:4H2O
Sylvite	-5.70	-4.87	0.83	KCl
Syngenite	-6.66	-14.26	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-37.75	-20.60	17.14	Mg2CaCl6:12H2O
Thenardite	-6.12	-6.48	-0.36	Na2SO4
Thermonatrite	-10.43	0.50	10.94	Na2CO3:H2O
Todorokite	-1.03	-46.85	-45.82	Mn7O12:3H2O
Trona-K	-18.15	-6.56	11.59	K2NaH(CO3)2:2H2O
Zincite	-2.05	9.15	11.20	ZnO
Zn	-50.60	18.19	68.79	Zn
Zn(ClO4)2:6H2O	-117.80	-112.16	5.63	Zn(ClO4)2:6H2O
Zn(g)	-67.22	18.19	85.41	Zn
Zn(OH)2(beta)	-2.78	9.15	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-2.51	9.15	11.66	Zn(OH)2
Zn(OH)2(gamma)	-2.73	9.15	11.88	Zn(OH)2
Zn2(OH)3Cl	-5.77	9.53	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-6.01	1.57	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-8.49	0.82	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-25.10	-6.01	19.09	Zn3O(SO4)2
ZnCl2	-15.49	-8.41	7.08	ZnCl2
ZnCO3:H2O	-0.74	-0.60	0.14	ZnCO3:H2O
ZnSO4	-11.11	-7.58	3.53	ZnSO4
ZnSO4:6H2O	-5.88	-7.58	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.71	-7.58	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-7.03	-7.58	-0.55	ZnSO4:H2O

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Beginning of batch-reaction calculations.  
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Reaction step 1.

Using mix 2.

Mixture 2.

1.000e+000 Solution 1 Flujo 2  
3.000e+000 Solution 3 AS2

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

Elements	Molality	Moles
Al	7.792e-005	3.117e-004
As	2.533e-006	1.013e-005
C	1.894e-003	7.575e-003
Ca	4.686e-003	1.874e-002
Cl	1.470e-002	5.881e-002
Cu	3.939e-007	1.575e-006
Fe	1.945e-004	7.780e-004
K	8.840e-004	3.536e-003
Mg	5.417e-004	2.167e-003
Mn	2.889e-005	1.156e-004
Na	1.300e-002	5.199e-002
S	5.810e-003	2.324e-002
Zn	3.378e-005	1.351e-004

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

pH = 5.800 Charge balance  
 pe = 13.852 Adjusted to redox equilibrium  
 Activity of water = 0.999  
 Ionic strength = 3.291e-002  
 Mass of water (kg) = 4.000e+000  
 Total alkalinity (eq/kg) = 7.040e-004  
 Total CO2 (mol/kg) = 1.894e-003  
 Temperature (deg C) = 25.000  
 Electrical balance (eq) = -8.544e-003  
 Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -4.51  
 Iterations = 9  
 Total H = 4.442122e+002  
 Total O = 2.222164e+002

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.816e-006	1.585e-006	-5.741	-5.800	-0.059
OH-	7.225e-009	6.073e-009	-8.141	-8.217	-0.075
H2O	5.553e+001	9.993e-001	1.744	-0.000	0.000
Al	7.792e-005				
Al13O4(OH)24+7	5.836e-006	2.628e-009	-5.234	-8.580	-3.347
AlOH+2	6.291e-007	3.217e-007	-6.201	-6.492	-0.291
Al(OH)2+	5.578e-007	4.709e-007	-6.253	-6.327	-0.074
HA1O2	4.323e-007	4.323e-007	-6.364	-6.364	0.000
Al+3	1.587e-007	4.556e-008	-6.799	-7.341	-0.542
AlSO4+	1.308e-007	1.105e-007	-6.883	-6.957	-0.074
AlO2-	1.107e-007	9.341e-008	-6.956	-7.030	-0.074
Al(SO4)2-	2.407e-008	2.032e-008	-7.619	-7.692	-0.074
Al2(OH)2+4	2.201e-010	1.683e-011	-9.657	-10.774	-1.116
NaAlO2	1.921e-010	1.921e-010	-9.717	-9.717	0.000
Al3(OH)4+5	1.001e-011	1.967e-013	-10.999	-12.706	-1.707
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-151.961	-151.961	0.000
As(3)	1.471e-029				
HAsO2	7.847e-030	7.847e-030	-29.105	-29.105	0.000
As(OH)3	6.857e-030	6.857e-030	-29.164	-29.164	0.000
H2AsO3-	3.133e-033	2.645e-033	-32.504	-32.578	-0.074
AsO2-	2.997e-033	2.530e-033	-32.523	-32.597	-0.074
AsO2OH-2	3.240e-038	1.630e-038	-37.490	-37.788	-0.298
HAsS2	0.000e+000	0.000e+000	-283.352	-283.352	0.000
As(5)	2.533e-006				
H2AsO4-	2.154e-006	1.818e-006	-5.667	-5.740	-0.074
HAsO4-2	3.784e-007	1.904e-007	-6.422	-6.720	-0.298
H3AsO4	5.077e-010	5.077e-010	-9.294	-9.294	0.000
AsO4-3	1.450e-012	3.081e-013	-11.839	-12.511	-0.673
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-250.670	-250.670	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-221.086	-221.086	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-138.523	-138.523	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.190	-47.190	0.000
C(4)	1.894e-003				
CO2	1.415e-003	1.427e-003	-2.849	-2.846	0.003
HCO3-	4.593e-004	3.877e-004	-3.338	-3.411	-0.074
CaHCO3+	1.146e-005	9.676e-006	-4.941	-5.014	-0.074
NaHCO3	5.978e-006	5.978e-006	-5.223	-5.223	0.000
MgHCO3+	1.190e-006	1.005e-006	-5.924	-5.998	-0.074
ZnHCO3+	1.662e-007	1.403e-007	-6.779	-6.853	-0.074
CaCO3	5.296e-008	5.296e-008	-7.276	-7.276	0.000

MnHCO3+	4.058e-008	3.426e-008	-7.392	-7.465	-0.074
CO3-2	2.122e-008	1.085e-008	-7.673	-7.965	-0.291
CuCO3	1.571e-008	1.571e-008	-7.804	-7.804	0.000
FeCO3+	1.141e-008	9.636e-009	-7.943	-8.016	-0.074
MnCO3	4.408e-009	4.408e-009	-8.356	-8.356	0.000
MgCO3	2.561e-009	2.561e-009	-8.592	-8.592	0.000
ZnCO3	1.279e-009	1.279e-009	-8.893	-8.893	0.000
NaCO3-	4.847e-010	4.092e-010	-9.315	-9.388	-0.074
FeHCO3+	5.441e-012	4.593e-012	-11.264	-11.338	-0.074
Cu(CO3)2-2	6.033e-013	3.036e-013	-12.219	-12.518	-0.298
FeCO3	1.391e-014	1.391e-014	-13.857	-13.857	0.000
CuCO3(OH)2-2	1.054e-016	5.306e-017	-15.977	-16.275	-0.298
Ca	4.686e-003				
Ca+2	3.939e-003	2.106e-003	-2.405	-2.677	-0.272
CaSO4	7.289e-004	7.289e-004	-3.137	-3.137	0.000
CaHCO3+	1.146e-005	9.676e-006	-4.941	-5.014	-0.074
CaCl+	6.490e-006	5.479e-006	-5.188	-5.261	-0.074
CaCl2	7.910e-008	7.910e-008	-7.102	-7.102	0.000
CaCO3	5.296e-008	5.296e-008	-7.276	-7.276	0.000
CaOH+	2.221e-010	1.875e-010	-9.653	-9.727	-0.074
Cl(-1)	1.470e-002				
Cl-	1.467e-002	1.227e-002	-1.834	-1.911	-0.077
NaCl	2.325e-005	2.325e-005	-4.634	-4.634	0.000
CaCl+	6.490e-006	5.479e-006	-5.188	-5.261	-0.074
MgCl+	2.533e-006	2.139e-006	-5.596	-5.670	-0.074
MnCl+	3.593e-007	3.033e-007	-6.445	-6.518	-0.074
ZnCl+	3.430e-007	2.896e-007	-6.465	-6.538	-0.074
KCl	2.992e-007	2.992e-007	-6.524	-6.524	0.000
CaCl2	7.910e-008	7.910e-008	-7.102	-7.102	0.000
CuCl+	6.036e-009	5.095e-009	-8.219	-8.293	-0.074
HCl	4.371e-009	4.371e-009	-8.359	-8.359	0.000
ZnCl2	4.152e-009	4.152e-009	-8.382	-8.382	0.000
Zn(OH)Cl	3.121e-009	3.121e-009	-8.506	-8.506	0.000
ZnCl3-	3.334e-011	2.814e-011	-10.477	-10.551	-0.074
CuCl2	3.294e-011	3.294e-011	-10.482	-10.482	0.000
MnCl3-	1.183e-011	9.983e-012	-10.927	-11.001	-0.074
ZnCl4-2	5.204e-012	2.619e-012	-11.284	-11.582	-0.298
FeCl2+	3.702e-012	3.125e-012	-11.432	-11.505	-0.074
FeCl+2	6.150e-013	3.145e-013	-12.211	-12.502	-0.291
FeCl+	2.391e-013	2.019e-013	-12.621	-12.695	-0.074
CuCl2-	1.383e-017	1.167e-017	-16.859	-16.933	-0.074
FeCl2	1.330e-017	1.330e-017	-16.876	-16.876	0.000
CuCl3-2	1.829e-018	9.202e-019	-17.738	-18.036	-0.298
FeCl4-	6.707e-019	5.662e-019	-18.173	-18.247	-0.074
CuCl4-2	1.851e-019	9.314e-020	-18.733	-19.031	-0.298
FeCl4-2	1.150e-020	5.789e-021	-19.939	-20.237	-0.298
Cl(1)	1.151e-019				
HClO	1.128e-019	1.128e-019	-18.948	-18.948	0.000
ClO-	2.273e-021	1.919e-021	-20.643	-20.717	-0.074
Cl(3)	4.540e-033				
ClO2-	4.531e-033	3.825e-033	-32.344	-32.417	-0.074
HClO2	8.965e-036	8.965e-036	-35.047	-35.047	0.000
Cl(5)	6.454e-031				
ClO3-	6.454e-031	5.425e-031	-30.190	-30.266	-0.075
Cl(7)	4.570e-033				
ClO4-	4.568e-033	3.840e-033	-32.340	-32.416	-0.075
ZnClO4+	1.208e-036	1.020e-036	-35.918	-35.991	-0.074
Cu(1)	1.704e-017				
CuCl2-	1.383e-017	1.167e-017	-16.859	-16.933	-0.074
CuCl3-2	1.829e-018	9.202e-019	-17.738	-18.036	-0.298
Cu+	1.385e-018	1.169e-018	-17.859	-17.932	-0.074
Cu(2)	3.939e-007				
Cu+2	2.839e-007	1.518e-007	-6.547	-6.819	-0.272
CuSO4	8.237e-008	8.237e-008	-7.084	-7.084	0.000
CuCO3	1.571e-008	1.571e-008	-7.804	-7.804	0.000
CuCl+	6.036e-009	5.095e-009	-8.219	-8.293	-0.074
CuOH+	5.845e-009	4.934e-009	-8.233	-8.307	-0.074

CuCl2	3.294e-011	3.294e-011	-10.482	-10.482	0.000
Cu(CO3)2-2	6.033e-013	3.036e-013	-12.219	-12.518	-0.298
CuCO3(OH)2-2	1.054e-016	5.306e-017	-15.977	-16.275	-0.298
CuCl4-2	1.851e-019	9.314e-020	-18.733	-19.031	-0.298
CuO2-2	1.693e-023	8.519e-024	-22.771	-23.070	-0.298
Fe(2)	5.640e-011				
Fe+2	4.222e-011	2.257e-011	-10.374	-10.646	-0.272
FeSO4	8.476e-012	8.476e-012	-11.072	-11.072	0.000
FeHCO3+	5.441e-012	4.593e-012	-11.264	-11.338	-0.074
FeCl+	2.391e-013	2.019e-013	-12.621	-12.695	-0.074
FeCO3	1.391e-014	1.391e-014	-13.857	-13.857	0.000
FeOH+	5.330e-015	4.500e-015	-14.273	-14.347	-0.074
FeCl2	1.330e-017	1.330e-017	-16.876	-16.876	0.000
Fe(OH)2	2.253e-020	2.253e-020	-19.647	-19.647	0.000
FeCl4-2	1.150e-020	5.789e-021	-19.939	-20.237	-0.298
Fe(OH)3-	6.697e-025	5.654e-025	-24.174	-24.248	-0.074
Fe(OH)4-2	7.083e-034	3.564e-034	-33.150	-33.448	-0.298
Fe(3)	1.945e-004				
Fe(OH)2+	1.547e-004	1.306e-004	-3.810	-3.884	-0.074
Fe(OH)3	3.851e-005	3.851e-005	-4.414	-4.414	0.000
FeOH+2	1.224e-006	6.258e-007	-5.912	-6.204	-0.291
FeCO3+	1.141e-008	9.636e-009	-7.943	-8.016	-0.074
Fe(OH)4-	7.224e-009	6.098e-009	-8.141	-8.215	-0.074
Fe+3	5.356e-010	1.538e-010	-9.271	-9.813	-0.542
Fe2(OH)2+4	1.378e-010	1.054e-011	-9.861	-10.977	-1.116
FeSO4+	4.176e-011	3.525e-011	-10.379	-10.453	-0.074
Fe3(OH)4+5	1.465e-011	2.877e-013	-10.834	-12.541	-1.707
FeCl2+	3.702e-012	3.125e-012	-11.432	-11.505	-0.074
Fe(SO4)2-	1.673e-012	1.412e-012	-11.777	-11.850	-0.074
FeCl+2	6.150e-013	3.145e-013	-12.211	-12.502	-0.291
FeCl4-	6.707e-019	5.662e-019	-18.173	-18.247	-0.074
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-42.407	-42.403	0.003
K	8.840e-004				
K+	8.672e-004	7.257e-004	-3.062	-3.139	-0.077
KSO4-	1.644e-005	1.388e-005	-4.784	-4.858	-0.074
KCl	2.992e-007	2.992e-007	-6.524	-6.524	0.000
KHSO4	1.941e-011	1.941e-011	-10.712	-10.712	0.000
KOH	1.586e-012	1.586e-012	-11.800	-11.800	0.000
Mg	5.417e-004				
Mg+2	3.968e-004	2.232e-004	-3.401	-3.651	-0.250
MgSO4	1.412e-004	1.412e-004	-3.850	-3.850	0.000
MgCl+	2.533e-006	2.139e-006	-5.596	-5.670	-0.074
MgHCO3+	1.190e-006	1.005e-006	-5.924	-5.998	-0.074
MgCO3	2.561e-009	2.561e-009	-8.592	-8.592	0.000
Mg4(OH)4+4	9.106e-031	6.965e-032	-30.041	-31.157	-1.116
Mn(2)	2.889e-005				
Mn+2	2.171e-005	1.160e-005	-4.663	-4.935	-0.272
MnSO4	6.784e-006	6.784e-006	-5.169	-5.169	0.000
MnCl+	3.593e-007	3.033e-007	-6.445	-6.518	-0.074
MnHCO3+	4.058e-008	3.426e-008	-7.392	-7.465	-0.074
MnCO3	4.408e-009	4.408e-009	-8.356	-8.356	0.000
MnOH+	2.227e-010	1.880e-010	-9.652	-9.726	-0.074
MnCl3-	1.183e-011	9.983e-012	-10.927	-11.001	-0.074
Mn2OH+3	1.025e-014	2.338e-015	-13.989	-14.631	-0.642
Mn(OH)2	2.909e-016	2.909e-016	-15.536	-15.536	0.000
Mn2(OH)3+	5.030e-017	4.246e-017	-16.298	-16.372	-0.074
Mn(OH)3-	2.038e-022	1.720e-022	-21.691	-21.764	-0.074
Mn(OH)4-2	1.825e-030	9.182e-031	-29.739	-30.037	-0.298
Mn(3)	9.640e-017				
Mn+3	9.640e-017	2.199e-017	-16.016	-16.658	-0.642
Mn(6)	5.250e-022				
MnO4-2	5.250e-022	2.642e-022	-21.280	-21.578	-0.298
Mn(7)	9.832e-018				
MnO4-	9.832e-018	8.264e-018	-17.007	-17.083	-0.075
Na	1.300e-002				
Na+	1.277e-002	1.078e-002	-1.894	-1.967	-0.074

NaSO4-	1.999e-004	1.687e-004	-3.699	-3.773	-0.074
NaCl	2.325e-005	2.325e-005	-4.634	-4.634	0.000
NaHCO3	5.978e-006	5.978e-006	-5.223	-5.223	0.000
NaCO3-	4.847e-010	4.092e-010	-9.315	-9.388	-0.074
NaAlO2	1.921e-010	1.921e-010	-9.717	-9.717	0.000
NaOH	1.129e-011	1.129e-011	-10.947	-10.947	0.000
O(0)	8.085e-008				
O2	4.043e-008	4.075e-008	-7.393	-7.390	0.003
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-130.718	-130.718	0.000
HS-	0.000e+000	0.000e+000	-131.853	-131.928	-0.075
S-2	0.000e+000	0.000e+000	-138.770	-139.054	-0.285
S2-2	0.000e+000	0.000e+000	-233.995	-234.293	-0.298
HAsS2	0.000e+000	0.000e+000	-283.352	-283.352	0.000
S3-2	0.000e+000	0.000e+000	-329.275	-329.574	-0.298
S4-2	0.000e+000	0.000e+000	-424.783	-425.081	-0.298
S5-2	0.000e+000	0.000e+000	-520.507	-520.805	-0.298
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-135.246	-135.544	-0.298
HS2O3-	0.000e+000	0.000e+000	-140.257	-140.330	-0.074
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-123.883	-124.167	-0.285
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-44.043	-44.117	-0.074
SO3-2	0.000e+000	0.000e+000	-45.257	-45.548	-0.291
H2SO3	0.000e+000	0.000e+000	-47.935	-47.935	0.000
SO2	0.000e+000	0.000e+000	-48.035	-48.035	0.000
S2O6-2	0.000e+000	0.000e+000	-64.226	-64.524	-0.298
S3O6-2	0.000e+000	0.000e+000	-161.989	-162.287	-0.298
S4O6-2	0.000e+000	0.000e+000	-243.846	-244.145	-0.298
S5O6-2	0.000e+000	0.000e+000	-354.583	-354.882	-0.298
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-92.765	-93.063	-0.298
S(6)	5.810e-003				
SO4-2	4.709e-003	2.369e-003	-2.327	-2.625	-0.298
CaSO4	7.289e-004	7.289e-004	-3.137	-3.137	0.000
NaSO4-	1.999e-004	1.687e-004	-3.699	-3.773	-0.074
MgSO4	1.412e-004	1.412e-004	-3.850	-3.850	0.000
KSO4-	1.644e-005	1.388e-005	-4.784	-4.858	-0.074
ZnSO4	6.990e-006	6.990e-006	-5.156	-5.156	0.000
MnSO4	6.784e-006	6.784e-006	-5.169	-5.169	0.000
HSO4-	4.494e-007	3.794e-007	-6.347	-6.421	-0.074
AlSO4+	1.308e-007	1.105e-007	-6.883	-6.957	-0.074
CuSO4	8.237e-008	8.237e-008	-7.084	-7.084	0.000
Al(SO4)2-	2.407e-008	2.032e-008	-7.619	-7.692	-0.074
FeSO4+	4.176e-011	3.525e-011	-10.379	-10.453	-0.074
KHSO4	1.941e-011	1.941e-011	-10.712	-10.712	0.000
FeSO4	8.476e-012	8.476e-012	-11.072	-11.072	0.000
Fe(SO4)2-	1.673e-012	1.412e-012	-11.777	-11.850	-0.074
H2SO4	5.675e-016	5.675e-016	-15.246	-15.246	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-42.702	-43.000	-0.298
S(8)	4.929e-030				
HSO5-	4.929e-030	4.161e-030	-29.307	-29.381	-0.074
Zn	3.378e-005				
Zn+2	2.626e-005	1.404e-005	-4.581	-4.853	-0.272
ZnSO4	6.990e-006	6.990e-006	-5.156	-5.156	0.000
ZnCl+	3.430e-007	2.896e-007	-6.465	-6.538	-0.074
ZnHCO3+	1.662e-007	1.403e-007	-6.779	-6.853	-0.074
ZnOH+	1.150e-008	9.706e-009	-7.939	-8.013	-0.074
ZnCl2	4.152e-009	4.152e-009	-8.382	-8.382	0.000
Zn(OH)Cl	3.121e-009	3.121e-009	-8.506	-8.506	0.000
ZnCO3	1.279e-009	1.279e-009	-8.893	-8.893	0.000
ZnCl3-	3.334e-011	2.814e-011	-10.477	-10.551	-0.074
Zn(OH)2	2.620e-011	2.620e-011	-10.582	-10.582	0.000
ZnCl4-2	5.204e-012	2.619e-012	-11.284	-11.582	-0.298
Zn(OH)3-	6.064e-017	5.120e-017	-16.217	-16.291	-0.074

Zn(OH)4-2	1.093e-023	5.502e-024	-22.961	-23.259	-0.298
ZnClO4+	1.208e-036	1.020e-036	-35.918	-35.991	-0.074

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

Phase	SI	log IAP	log KT	
Al	-134.31	15.60	149.91	Al
Al(g)	-185.02	15.60	200.62	Al
Al2(SO4)3	-41.46	-22.56	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-24.12	-22.56	1.56	Al2(SO4)3:6H2O
Alabandite	-130.64	-131.06	-0.42	MnS
Alum-K	-10.76	-15.73	-4.97	KAl(SO4)2:12H2O
Alunite	4.85	4.38	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.95	-5.30	-4.35	CaSO4
Antarcticite	-10.59	-6.50	4.09	CaCl2:6H2O
Antlerite	-8.61	0.12	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.75	-16.64	-3.89	NaK3(SO4)2
Aragonite	-2.26	-0.29	1.97	CaCO3
Arcanite	-7.06	-8.90	-1.84	K2SO4
Arsenolite	-56.91	-76.75	-19.84	As2O3
Arsenopyrite	-217.50	-231.94	-14.45	FeAsS
Artinite	-12.94	6.68	19.63	Mg2CO3(OH)2:3H2O
As	-75.52	-32.83	42.68	As
As2O5	-25.22	-23.08	2.14	As2O5
As4O6(cubi)	-113.68	-153.51	-39.82	As4O6
As4O6(mono)	-113.46	-153.51	-40.05	As4O6
Atacamite	-10.56	3.70	14.26	Cu4Cl2(OH)6
Azurite	-13.20	-4.08	9.12	Cu3(CO3)2(OH)2
Bassanite	-1.60	-5.30	-3.71	CaSO4:0.5H2O
Birnessite	19.33	-66.21	-85.55	Mn8O14:5H2O
Bischofite	-11.87	-7.48	4.39	MgCl2:6H2O
Bixbyite	2.45	1.48	-0.96	Mn2O3
Bloedite	-10.36	-12.84	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	2.51	10.06	7.55	AlO2H
Bornite	-491.17	-593.71	-102.53	Cu5FeS4
Brochantite	-10.53	4.90	15.42	Cu4(SO4)(OH)6
Brucite	-8.34	7.95	16.28	Mg(OH)2
Burkeite	-24.15	-14.67	9.49	Na6CO3(SO4)2
C	-65.97	-1.82	64.15	C
C(g)	-183.59	-1.82	181.77	C
Ca	-127.21	12.62	139.83	Ca
Ca(g)	-152.45	12.62	165.07	Ca
Ca2Al2O5:8H2O	-21.61	37.96	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-23.87	2.42	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-14.11	3.69	17.80	Ca3(AsO4)2
Ca3Al2O6	-66.15	46.88	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-69.50	70.98	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-51.45	55.80	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-47.88	55.80	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-48.06	20.27	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-17.87	29.04	46.91	CaAl2O4
CaAl2O4:10H2O	-8.96	29.04	37.99	CaAl2O4:10H2O
CaAl4O7	-19.44	49.15	68.59	CaAl4O7
Calcite	-2.11	-0.29	1.82	CaCO3
Carnallite	-16.80	-12.53	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.77	-5.30	-3.54	CaSO4:0.5H2O
CH4(g)	-135.68	-138.52	-2.84	CH4
Chalcanthite	-6.82	-9.45	-2.63	CuSO4:5H2O
Chalcocite	-127.25	-161.99	-34.74	Cu2S
Chalcocyanite	-12.36	-9.44	2.91	CuSO4
Chalcopyrite	-237.12	-269.72	-32.60	CuFeS2
Chloromagnesite	-29.29	-7.47	21.82	MgCl2
Cl2(g)	-22.11	-19.12	2.99	Cl2
Claudetite	-56.96	-76.75	-19.80	As2O3
CO(g)	-44.19	-47.19	-3.00	CO
CO2(g)	-1.38	-9.21	-7.83	CO2

Corundum	1.82	20.12	18.29	Al <sub>2</sub> O <sub>3</sub>
Covellite	-110.09	-132.95	-22.86	CuS
Cu	-23.02	8.48	31.50	Cu
Cu(g)	-75.18	8.48	83.66	Cu
CuCl <sub>2</sub>	-14.36	-10.64	3.72	CuCl <sub>2</sub>
Cuprite	-22.36	-24.26	-1.91	Cu <sub>2</sub> O
Dawsonite	0.34	4.68	4.34	NaAlCO <sub>3</sub> (OH) <sub>2</sub>
Delafoosite	1.89	-4.55	-6.44	CuFeO <sub>2</sub>
Diaspore	2.91	10.06	7.15	AlHO <sub>2</sub>
Dolomite	-4.02	-1.55	2.47	CaMg(CO <sub>3</sub> ) <sub>2</sub>
Dolomite-dis	-5.56	-1.55	4.01	CaMg(CO <sub>3</sub> ) <sub>2</sub>
Dolomite-ord	-4.02	-1.55	2.46	CaMg(CO <sub>3</sub> ) <sub>2</sub>
Epsomite	-4.32	-6.28	-1.96	MgSO <sub>4</sub> ·7H <sub>2</sub> O
Ettringite	-31.49	30.97	62.46	Ca <sub>6</sub> Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> (OH) <sub>12</sub> ·26H <sub>2</sub> O
Fe	-54.37	4.65	59.02	Fe
Fe(OH) <sub>2</sub>	-12.94	0.95	13.89	Fe(OH) <sub>2</sub>
Fe(OH) <sub>3</sub>	1.95	7.59	5.64	Fe(OH) <sub>3</sub>
Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	-30.55	-27.50	3.05	Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>
FeO	-12.57	0.95	13.52	FeO
Ferrite-Ca	2.60	24.10	21.50	CaFe <sub>2</sub> O <sub>4</sub>
Ferrite-Cu	9.67	19.95	10.28	CuFe <sub>2</sub> O <sub>4</sub>
Ferrite-Dicalcium	-23.78	33.02	56.80	Ca <sub>2</sub> Fe <sub>2</sub> O <sub>5</sub>
Ferrite-Mg	2.10	23.12	21.02	MgFe <sub>2</sub> O <sub>4</sub>
Ferrite-Zn	10.22	21.92	11.70	ZnFe <sub>2</sub> O <sub>4</sub>
FeSO <sub>4</sub>	-15.88	-13.27	2.61	FeSO <sub>4</sub>
Gaylussite	-13.00	-1.84	11.16	CaNa <sub>2</sub> (CO <sub>3</sub> ) <sub>2</sub> ·5H <sub>2</sub> O
Gibbsite	2.32	10.06	7.74	Al(OH) <sub>3</sub>
Glauberite	-6.39	-11.86	-5.47	Na <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub>
Goethite	7.06	7.59	0.53	FeOOH
Gypsum	-0.77	-5.30	-4.53	CaSO <sub>4</sub> ·2H <sub>2</sub> O
H <sub>2</sub> (g)	-39.30	-42.40	-3.10	H <sub>2</sub>
H <sub>2</sub> O(g)	-1.59	-0.00	1.59	H <sub>2</sub> O
H <sub>2</sub> S(g)	-129.74	-137.73	-7.99	H <sub>2</sub> S
Halite	-5.44	-3.88	1.56	NaCl
Hausmannite	-2.00	8.15	10.14	Mn <sub>3</sub> O <sub>4</sub>
HCl(g)	-14.01	-7.71	6.30	HCl
Hematite	15.10	15.17	0.08	Fe <sub>2</sub> O <sub>3</sub>
Hercynite	-7.73	21.07	28.80	FeAl <sub>2</sub> O <sub>4</sub>
Hexahydrite	-4.55	-6.28	-1.73	MgSO <sub>4</sub> ·6H <sub>2</sub> O
Huntite	-14.29	-4.08	10.22	CaMg <sub>3</sub> (CO <sub>3</sub> ) <sub>4</sub>
Hydromagnesite	-27.84	2.89	30.74	Mg <sub>5</sub> (CO <sub>3</sub> ) <sub>4</sub> (OH) <sub>2</sub> ·4H <sub>2</sub> O
Hydrophilite	-18.24	-6.50	11.75	CaCl <sub>2</sub>
Hydrozincite	-15.00	15.31	30.31	Zn <sub>5</sub> (OH) <sub>6</sub> (CO <sub>3</sub> ) <sub>2</sub>
Ice	-0.14	-0.00	0.14	H <sub>2</sub> O
Jarosite	6.38	-3.03	-9.41	KFe <sub>3</sub> (SO <sub>4</sub> ) <sub>2</sub> (OH) <sub>6</sub>
Jarosite-Na	3.59	-1.86	-5.45	NaFe <sub>3</sub> (SO <sub>4</sub> ) <sub>2</sub> (OH) <sub>6</sub>
K	-66.47	4.51	70.98	K
K(g)	-77.07	4.51	81.58	K
K <sub>2</sub> CO <sub>3</sub> ·1.5H <sub>2</sub> O	-17.27	-3.89	13.38	K <sub>2</sub> CO <sub>3</sub> ·1.5H <sub>2</sub> O
K <sub>2</sub> O	-78.71	5.32	84.04	K <sub>2</sub> O
K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>	-16.84	-20.47	-3.62	K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>
K <sub>8</sub> H <sub>4</sub> (CO <sub>3</sub> ) <sub>6</sub> ·3H <sub>2</sub> O	-61.69	-33.98	27.71	K <sub>8</sub> H <sub>4</sub> (CO <sub>3</sub> ) <sub>6</sub> ·3H <sub>2</sub> O
Kainite	-11.02	-11.33	-0.31	KMgClSO <sub>4</sub> ·3H <sub>2</sub> O
KAl(SO <sub>4</sub> ) <sub>2</sub>	-19.00	-15.73	3.27	KAl(SO <sub>4</sub> ) <sub>2</sub>
Kalinite	-6.83	-6.55	0.28	KHCO <sub>3</sub>
Katoite	-32.06	46.88	78.94	Ca <sub>3</sub> Al <sub>2</sub> H <sub>12</sub> O <sub>12</sub>
Kieserite	-6.01	-6.28	-0.27	MgSO <sub>4</sub> ·H <sub>2</sub> O
KMgCl <sub>3</sub>	-33.77	-12.52	21.25	KMgCl <sub>3</sub>
KMgCl <sub>3</sub> ·2H <sub>2</sub> O	-26.49	-12.52	13.96	KMgCl <sub>3</sub> ·2H <sub>2</sub> O
KNaCO <sub>3</sub> ·6H <sub>2</sub> O	-12.98	-2.72	10.26	KNaCO <sub>3</sub> ·6H <sub>2</sub> O
Lammerite	-10.29	-8.74	1.55	Cu <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>
Lansfordite	-6.11	-1.26	4.84	MgCO <sub>3</sub> ·5H <sub>2</sub> O
Lawrencite	-23.52	-14.47	9.05	FeCl <sub>2</sub>
Leonite	-11.07	-15.18	-4.11	K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> ·4H <sub>2</sub> O
Lime	-23.65	8.92	32.57	CaO
Magnesite	-3.54	-1.26	2.27	MgCO <sub>3</sub>
Magnetite	5.71	16.13	10.42	Fe <sub>3</sub> O <sub>4</sub>

Malachite	-5.55	0.35	5.90	$\text{Cu}_2\text{CO}_3(\text{OH})_2$
Manganite	0.91	0.74	-0.16	$\text{MnO}(\text{OH})$
Manganosite	-11.25	6.66	17.92	MnO
Mayenite	-246.27	247.88	494.15	$\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$
Melanterite	-10.88	-13.27	-2.40	$\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$
Mercallite	-10.13	-11.56	-1.44	$\text{KHSO}_4$
Mg	-110.88	11.64	122.52	Mg
Mg(g)	-130.60	11.64	142.25	Mg
$\text{Mg}_{1.25}\text{SO}_4(\text{OH})0.5:0.5\text{H}_2\text{O}$	-9.49	-4.29	5.20	$\text{Mg}_{1.25}\text{SO}_4(\text{OH})0.5:0.5\text{H}_2\text{O}$
$\text{Mg}_{1.5}\text{SO}_4(\text{OH})$	-11.51	-2.30	9.21	$\text{Mg}_{1.5}\text{SO}_4(\text{OH})$
$\text{MgCl}_2:2\text{H}_2\text{O}$	-20.21	-7.47	12.73	$\text{MgCl}_2:2\text{H}_2\text{O}$
$\text{MgCl}_2:4\text{H}_2\text{O}$	-14.78	-7.47	7.30	$\text{MgCl}_2:4\text{H}_2\text{O}$
$\text{MgCl}_2:\text{H}_2\text{O}$	-23.55	-7.47	16.07	$\text{MgCl}_2:\text{H}_2\text{O}$
MgOHCl	-15.65	0.24	15.89	MgOHCl
MgSO <sub>4</sub>	-11.10	-6.28	4.83	MgSO <sub>4</sub>
Mirabilite	-5.41	-6.56	-1.15	$\text{Na}_2\text{SO}_4:10\text{H}_2\text{O}$
Misenite	-67.21	-78.29	-11.08	$\text{K}_8\text{H}_6(\text{SO}_4)_7$
Mn	-72.57	10.36	82.93	Mn
$\text{Mn}(\text{OH})_2(\text{am})$	-8.64	6.66	15.31	$\text{Mn}(\text{OH})_2$
$\text{Mn}(\text{OH})_3$	-5.60	0.74	6.34	$\text{Mn}(\text{OH})_3$
$\text{MnCl}_2:2\text{H}_2\text{O}$	-12.76	-8.76	4.00	$\text{MnCl}_2:2\text{H}_2\text{O}$
$\text{MnCl}_2:4\text{H}_2\text{O}$	-11.51	-8.76	2.75	$\text{MnCl}_2:4\text{H}_2\text{O}$
$\text{MnCl}_2:\text{H}_2\text{O}$	-14.30	-8.76	5.54	$\text{MnCl}_2:\text{H}_2\text{O}$
$\text{MnO}_2(\text{gamma})$	2.87	-13.26	-16.13	MnO <sub>2</sub>
MnSO <sub>4</sub>	-10.17	-7.56	2.61	MnSO <sub>4</sub>
Molysite	-29.02	-15.55	13.47	$\text{FeCl}_3$
Monohydrocalcite	-2.97	-0.29	2.68	$\text{CaCO}_3:\text{H}_2\text{O}$
Na	-61.69	5.68	67.37	Na
Na(g)	-75.18	5.68	80.86	Na
$\text{Na}_2\text{CO}_3$	-12.71	-1.55	11.16	$\text{Na}_2\text{CO}_3$
$\text{Na}_2\text{CO}_3:7\text{H}_2\text{O}$	-11.49	-1.55	9.94	$\text{Na}_2\text{CO}_3:7\text{H}_2\text{O}$
Na <sub>2</sub> O	-59.75	7.66	67.42	Na <sub>2</sub> O
$\text{Na}_3\text{H}(\text{SO}_4)_2$	-16.06	-16.95	-0.89	$\text{Na}_3\text{H}(\text{SO}_4)_2$
$\text{Na}_4\text{Ca}(\text{SO}_4)_3:2\text{H}_2\text{O}$	-12.53	-18.42	-5.89	$\text{Na}_4\text{Ca}(\text{SO}_4)_3:2\text{H}_2\text{O}$
NaFeO <sub>2</sub>	-8.47	11.42	19.88	NaFeO <sub>2</sub>
Nahcolite	-5.24	-5.38	-0.14	NaHCO <sub>3</sub>
Nantokite	-13.08	-19.84	-6.77	CuCl
Natron	-11.14	-1.55	9.59	$\text{Na}_2\text{CO}_3:10\text{H}_2\text{O}$
Nesquehonite	-6.55	-1.26	5.29	$\text{MgCO}_3:3\text{H}_2\text{O}$
O <sub>2</sub> (g)	-4.50	-7.39	-2.89	O <sub>2</sub>
Orpiment	-410.45	-489.94	-79.49	As <sub>2</sub> S <sub>3</sub>
Oxychloride-Mg	-17.65	8.18	25.83	$\text{Mg}_2\text{Cl}(\text{OH})_3:4\text{H}_2\text{O}$
Pentahydrite	-4.89	-6.28	-1.39	$\text{MgSO}_4:5\text{H}_2\text{O}$
Periclase	-13.38	7.95	21.33	MgO
Picromerite	-10.74	-15.18	-4.44	$\text{K}_2\text{Mg}(\text{SO}_4)_2:6\text{H}_2\text{O}$
Pirssonite	-13.16	-1.84	11.32	$\text{Na}_2\text{Ca}(\text{CO}_3)_2:2\text{H}_2\text{O}$
Polyhalite	-11.47	-25.79	-14.31	$\text{K}_2\text{MgCa}_2(\text{SO}_4)_4:2\text{H}_2\text{O}$
Portlandite	-13.62	8.92	22.55	$\text{Ca}(\text{OH})_2$
Pyrite	-218.93	-243.63	-24.70	FeS <sub>2</sub>
Pyrolusite	4.40	-13.26	-17.66	MnO <sub>2</sub>
Pyrrhotite	-133.04	-136.77	-3.74	FeS
Realgar	-159.57	-219.84	-60.28	AsS
Rhodochrosite	-2.33	-2.55	-0.22	MnCO <sub>3</sub>
S	-96.31	-141.42	-45.11	S
S <sub>2</sub> (g)	-206.52	-213.70	-7.19	S <sub>2</sub>
Scacchite	-17.50	-8.76	8.74	MnCl <sub>2</sub>
Siderite	-8.04	-8.26	-0.22	FeCO <sub>3</sub>
Smithsonite	-2.91	-2.46	0.44	ZnCO <sub>3</sub>
SO <sub>2</sub> (g)	-48.21	-48.03	0.18	SO <sub>2</sub>
Sphalerite	-119.51	-130.98	-11.47	ZnS
Spinel	-9.54	28.06	37.61	Al <sub>2</sub> MgO <sub>4</sub>
Starkeyite	-5.28	-6.28	-1.00	$\text{MgSO}_4:4\text{H}_2\text{O}$
Sylvite	-5.88	-5.05	0.83	KCl
Syngenite	-6.61	-14.21	-7.60	$\text{K}_2\text{Ca}(\text{SO}_4)_2:\text{H}_2\text{O}$
Tachyhydrite	-38.59	-21.45	17.14	$\text{Mg}_2\text{CaCl}_6:12\text{H}_2\text{O}$
Tenorite	-2.87	4.78	7.65	CuO
Thenardite	-6.20	-6.56	-0.36	Na <sub>2</sub> SO <sub>4</sub>

Thermonatrite	-12.48	-1.55	10.94	Na2CO3:H2O
Todorokite	17.09	-28.73	-45.82	Mn7O12:3H2O
Troilite	-132.93	-136.77	-3.84	FeS
Trona-K	-20.86	-9.27	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-121.81	-130.98	-9.17	ZnS
Wustite	-10.80	1.61	12.40	Fe.947O
Zincite	-4.45	6.75	11.20	ZnO
Zn	-58.35	10.44	68.79	Zn
Zn(ClO4)2:6H2O	-75.32	-69.69	5.63	Zn(ClO4)2:6H2O
Zn(g)	-74.97	10.44	85.41	Zn
Zn(OH)2(beta)	-5.19	6.75	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-4.91	6.75	11.66	Zn(OH)2
Zn(OH)2(gamma)	-5.14	6.75	11.88	Zn(OH)2
Zn2(OH)3Cl	-9.51	5.78	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-8.31	-0.73	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-12.15	-2.84	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-27.30	-8.21	19.09	Zn3O(SO4)2
ZnCl2	-15.75	-8.67	7.08	ZnCl2
ZnCO3:H2O	-2.60	-2.46	0.14	ZnCO3:H2O
ZnSO4	-11.01	-7.48	3.53	ZnSO4
ZnSO4:6H2O	-5.78	-7.48	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.60	-7.48	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.93	-7.48	-0.55	ZnSO4:H2O

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End of simulation.  
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Reading input data for simulation 2.  
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End of run.  
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