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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 3  
temp 25  
pH 3.07  
pe 17  
redox pe  
units mg/l  
density 1  
Cl 40.91  
S(6) 1264  
Al 21.6  
As 3.82  
Ca 124.8  
Cu 40.91  
Fe 41.51  
K 35.01  
Mg 13.42  
Mn 24.26  
Na 20.89  
Zn 9.71  
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

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4      1
SELECTED_OUTPUT
file      DAM_AGUASUP
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 3

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

Elements	Molality	Moles
Al	8.019e-004	8.019e-004
As	5.107e-005	5.107e-005
Ca	3.119e-003	3.119e-003
Cl	1.156e-003	1.156e-003
Cu	6.448e-004	6.448e-004
Fe	7.445e-004	7.445e-004
K	8.969e-004	8.969e-004
Mg	5.531e-004	5.531e-004
Mn	4.423e-004	4.423e-004
Na	9.102e-004	9.102e-004
S(6)	1.318e-002	1.318e-002
Zn	1.487e-004	1.487e-004

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

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pH = 3.070
pe = 17.000
Activity of water = 1.000
Ionic strength = 3.218e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -2.266e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.053e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -30.80
Iterations = 8
Total H = 1.110530e+002
Total O = 5.557899e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	9.741e-004	8.511e-004	-3.011	-3.070	-0.059
OH-	1.344e-011	1.132e-011	-10.872	-10.946	-0.075
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	8.019e-004				
AlSO4+	4.097e-004	3.464e-004	-3.388	-3.460	-0.073
Al+3	2.262e-004	6.552e-005	-3.646	-4.184	-0.538
Al(SO4)2-	1.643e-004	1.389e-004	-3.784	-3.857	-0.073
AlOH+2	1.676e-006	8.621e-007	-5.776	-6.064	-0.289
Al(OH)2+	2.781e-009	2.351e-009	-8.556	-8.629	-0.073
Al2(OH)2+4	1.546e-009	1.208e-010	-8.811	-9.918	-1.107
HALO2	4.020e-012	4.020e-012	-11.396	-11.396	0.000
Al3(OH)4+5	3.475e-013	7.050e-015	-12.459	-14.152	-1.693
AlO2-	1.914e-015	1.618e-015	-14.718	-14.791	-0.073
NaAlO2	2.296e-019	2.296e-019	-18.639	-18.639	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-51.563	-54.881	-3.319

As(-3)	0.000e+000					
AsH3	0.000e+000	0.000e+000	-151.256	-151.256	0.000	
As(3)	2.419e-026					
HAsO2	1.291e-026	1.291e-026	-25.889	-25.889	0.000	
As(OH)3	1.128e-026	1.128e-026	-25.948	-25.948	0.000	
H2AsO3-	9.588e-033	8.107e-033	-32.018	-32.091	-0.073	
AsO2-	9.170e-033	7.753e-033	-32.038	-32.111	-0.073	
AsO2OH-2	1.838e-040	0.000e+000	-39.736	-40.031	-0.296	
As(5)	5.107e-005					
H2AsO4-	4.531e-005	3.831e-005	-4.344	-4.417	-0.073	
H3AsO4	5.743e-006	5.743e-006	-5.241	-5.241	0.000	
HAsO4-2	1.476e-008	7.471e-009	-7.831	-8.127	-0.296	
AsO4-3	1.045e-016	2.252e-017	-15.981	-16.647	-0.667	
Ca	3.119e-003					
Ca+2	2.219e-003	1.192e-003	-2.654	-2.924	-0.270	
CaSO4	8.999e-004	8.999e-004	-3.046	-3.046	0.000	
CaCl+	2.891e-007	2.445e-007	-6.539	-6.612	-0.073	
CaCl2	2.781e-010	2.781e-010	-9.556	-9.556	0.000	
CaOH+	2.340e-013	1.978e-013	-12.631	-12.704	-0.073	
Cl(-1)	1.156e-003					
Cl-	1.154e-003	9.673e-004	-2.938	-3.014	-0.077	
CuCl+	6.621e-007	5.598e-007	-6.179	-6.252	-0.073	
MnCl+	3.434e-007	2.903e-007	-6.464	-6.537	-0.073	
CaCl+	2.891e-007	2.445e-007	-6.539	-6.612	-0.073	
HCl	1.849e-007	1.849e-007	-6.733	-6.733	0.000	
MgCl+	1.568e-007	1.326e-007	-6.805	-6.878	-0.073	
NaCl	1.265e-007	1.265e-007	-6.898	-6.898	0.000	
ZnCl+	9.697e-008	8.198e-008	-7.013	-7.086	-0.073	
KCl	2.345e-008	2.345e-008	-7.630	-7.630	0.000	
FeCl+2	9.839e-009	5.061e-009	-8.007	-8.296	-0.289	
FeCl2+	4.688e-009	3.963e-009	-8.329	-8.402	-0.073	
CuCl2	2.852e-010	2.852e-010	-9.545	-9.545	0.000	
CaCl2	2.781e-010	2.781e-010	-9.556	-9.556	0.000	
ZnCl2	9.263e-011	9.263e-011	-10.033	-10.033	0.000	
FeCl+	2.730e-012	2.308e-012	-11.564	-11.637	-0.073	
Zn(OH)Cl	1.646e-012	1.646e-012	-11.783	-11.783	0.000	
MnCl3-	7.018e-014	5.934e-014	-13.154	-13.227	-0.073	
ZnCl3-	5.853e-014	4.948e-014	-13.233	-13.306	-0.073	
ZnCl4-2	7.166e-016	3.628e-016	-15.145	-15.440	-0.296	
FeCl2	1.198e-017	1.198e-017	-16.922	-16.922	0.000	
FeCl4-	5.273e-018	4.458e-018	-17.278	-17.351	-0.073	
CuCl2-	8.492e-020	7.180e-020	-19.071	-19.144	-0.073	
CuCl4-2	9.890e-021	5.007e-021	-20.005	-20.300	-0.296	
CuCl3-2	8.809e-022	4.460e-022	-21.055	-21.351	-0.296	
FeCl4-2	6.397e-023	3.239e-023	-22.194	-22.490	-0.296	
Cl(1)	3.282e-017					
HClO	3.282e-017	3.282e-017	-16.484	-16.484	0.000	
ClO-	1.230e-021	1.040e-021	-20.910	-20.983	-0.073	
Cl(3)	3.477e-032					
HClO2	1.792e-032	1.792e-032	-31.747	-31.747	0.000	
ClO2-	1.685e-032	1.424e-032	-31.773	-31.846	-0.073	
Cl(5)	1.650e-029					
ClO3-	1.650e-029	1.389e-029	-28.783	-28.857	-0.075	
Cl(7)	8.035e-031					
ClO4-	8.027e-031	6.758e-031	-30.095	-30.170	-0.075	
ZnClO4+	7.628e-034	6.449e-034	-33.118	-33.191	-0.073	
Cu(1)	1.456e-018					
Cu+	1.370e-018	1.158e-018	-17.863	-17.936	-0.073	
CuCl2-	8.492e-020	7.180e-020	-19.071	-19.144	-0.073	
CuCl3-2	8.809e-022	4.460e-022	-21.055	-21.351	-0.296	
Cu(2)	6.448e-004					
Cu+2	3.937e-004	2.116e-004	-3.405	-3.675	-0.270	
CuSO4	2.504e-004	2.504e-004	-3.601	-3.601	0.000	
CuCl+	6.621e-007	5.598e-007	-6.179	-6.252	-0.073	
CuOH+	1.516e-008	1.282e-008	-7.819	-7.892	-0.073	
CuCl2	2.852e-010	2.852e-010	-9.545	-9.545	0.000	
CuCl4-2	9.890e-021	5.007e-021	-20.005	-20.300	-0.296	

CuO2-2	2.825e-031	1.430e-031	-30.549	-30.845	-0.296
Fe(2)	8.779e-009				
Fe+2	6.095e-009	3.275e-009	-8.215	-8.485	-0.270
FeSO4	2.682e-009	2.682e-009	-8.572	-8.572	0.000
FeCl+	2.730e-012	2.308e-012	-11.564	-11.637	-0.073
FeOH+	1.439e-015	1.216e-015	-14.842	-14.915	-0.073
FeCl2	1.198e-017	1.198e-017	-16.922	-16.922	0.000
FeCl4-2	6.397e-023	3.239e-023	-22.194	-22.490	-0.296
Fe(OH)2	1.135e-023	1.135e-023	-22.945	-22.945	0.000
Fe(OH)3-	6.276e-031	5.306e-031	-30.202	-30.275	-0.073
Fe(OH)4-2	0.000e+000	0.000e+000	-41.910	-42.205	-0.296
Fe(3)	7.445e-004				
FeOH+2	4.629e-004	2.381e-004	-3.335	-3.623	-0.289
Fe(OH)2+	1.095e-004	9.261e-005	-3.960	-4.033	-0.073
Fe+3	1.084e-004	3.140e-005	-3.965	-4.503	-0.538
Fe2(OH)2+4	1.953e-005	1.526e-006	-4.709	-5.816	-1.107
FeSO4+	1.857e-005	1.570e-005	-4.731	-4.804	-0.073
Fe(SO4)2-	1.622e-006	1.371e-006	-5.790	-5.863	-0.073
Fe3(OH)4+5	1.455e-006	2.953e-008	-5.837	-7.530	-1.693
Fe(OH)3	5.087e-008	5.087e-008	-7.294	-7.294	0.000
FeCl+2	9.839e-009	5.061e-009	-8.007	-8.296	-0.289
FeCl2+	4.688e-009	3.963e-009	-8.329	-8.402	-0.073
Fe(OH)4-	1.775e-014	1.501e-014	-13.751	-13.824	-0.073
FeCl4-	5.273e-018	4.458e-018	-17.278	-17.351	-0.073
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.244	-43.240	0.003
K	8.969e-004				
K+	8.613e-004	7.219e-004	-3.065	-3.141	-0.077
KSO4-	3.561e-005	3.011e-005	-4.448	-4.521	-0.073
KCl	2.345e-008	2.345e-008	-7.630	-7.630	0.000
KHSO4	2.261e-008	2.261e-008	-7.646	-7.646	0.000
KOH	2.940e-015	2.940e-015	-14.532	-14.532	0.000
Mg	5.531e-004				
Mg+2	3.107e-004	1.755e-004	-3.508	-3.756	-0.248
MgSO4	2.422e-004	2.422e-004	-3.616	-3.616	0.000
MgCl+	1.568e-007	1.326e-007	-6.805	-6.878	-0.073
Mg4(OH)4+4	0.000e+000	0.000e+000	-41.386	-42.493	-1.107
Mn(2)	4.423e-004				
Mn+2	2.623e-004	1.410e-004	-3.581	-3.851	-0.270
MnSO4	1.797e-004	1.797e-004	-3.746	-3.746	0.000
MnCl+	3.434e-007	2.903e-007	-6.464	-6.537	-0.073
MnOH+	5.033e-012	4.255e-012	-11.298	-11.371	-0.073
MnCl3-	7.018e-014	5.934e-014	-13.154	-13.227	-0.073
Mn2OH+3	2.782e-015	6.427e-016	-14.556	-15.192	-0.636
Mn(OH)2	1.227e-020	1.227e-020	-19.911	-19.911	0.000
Mn2(OH)3+	4.793e-023	4.052e-023	-22.319	-22.392	-0.073
Mn(OH)3-	1.598e-029	1.351e-029	-28.796	-28.869	-0.073
Mn(OH)4-2	2.655e-040	1.344e-040	-39.576	-39.872	-0.296
Mn(3)	1.627e-012				
Mn+3	1.627e-012	3.760e-013	-11.789	-12.425	-0.636
Mn(6)	3.607e-030				
MnO4-2	3.607e-030	1.826e-030	-29.443	-29.738	-0.296
Mn(7)	9.551e-023				
MnO4-	9.551e-023	8.041e-023	-22.020	-22.095	-0.075
Na	9.102e-004				
Na+	8.800e-004	7.440e-004	-3.056	-3.128	-0.073
NaSO4-	3.004e-005	2.540e-005	-4.522	-4.595	-0.073
NaCl	1.265e-007	1.265e-007	-6.898	-6.898	0.000
NaOH	1.452e-015	1.452e-015	-14.838	-14.838	0.000
NaAlO2	2.296e-019	2.296e-019	-18.639	-18.639	0.000
O(0)	3.822e-006				
O2	1.911e-006	1.926e-006	-5.719	-5.715	0.003
S(6)	1.318e-002				
SO4-2	1.020e-002	5.166e-003	-1.991	-2.287	-0.296
CaSO4	8.999e-004	8.999e-004	-3.046	-3.046	0.000
HSO4-	5.254e-004	4.442e-004	-3.280	-3.352	-0.073
AlSO4+	4.097e-004	3.464e-004	-3.388	-3.460	-0.073

CuSO4	2.504e-004	2.504e-004	-3.601	-3.601	0.000
MgSO4	2.422e-004	2.422e-004	-3.616	-3.616	0.000
MnSO4	1.797e-004	1.797e-004	-3.746	-3.746	0.000
Al(SO4)2-	1.643e-004	1.389e-004	-3.784	-3.857	-0.073
ZnSO4	5.476e-005	5.476e-005	-4.262	-4.262	0.000
KSO4-	3.561e-005	3.011e-005	-4.448	-4.521	-0.073
NaSO4-	3.004e-005	2.540e-005	-4.522	-4.595	-0.073
FeSO4+	1.857e-005	1.570e-005	-4.731	-4.804	-0.073
Fe(SO4)2-	1.622e-006	1.371e-006	-5.790	-5.863	-0.073
KHSO4	2.261e-008	2.261e-008	-7.646	-7.646	0.000
FeSO4	2.682e-009	2.682e-009	-8.572	-8.572	0.000
H2SO4	3.567e-010	3.567e-010	-9.448	-9.448	0.000
Zn	1.487e-004				
Zn+2	9.388e-005	5.045e-005	-4.027	-4.297	-0.270
ZnSO4	5.476e-005	5.476e-005	-4.262	-4.262	0.000
ZnCl+	9.697e-008	8.198e-008	-7.013	-7.086	-0.073
ZnCl2	9.263e-011	9.263e-011	-10.033	-10.033	0.000
ZnOH+	7.685e-011	6.498e-011	-10.114	-10.187	-0.073
Zn(OH)Cl	1.646e-012	1.646e-012	-11.783	-11.783	0.000
ZnCl3-	5.853e-014	4.948e-014	-13.233	-13.306	-0.073
ZnCl4-2	7.166e-016	3.628e-016	-15.145	-15.440	-0.296
Zn(OH)2	3.268e-016	3.268e-016	-15.486	-15.486	0.000
Zn(OH)3-	1.407e-024	1.190e-024	-23.852	-23.925	-0.073
ZnClO4+	7.628e-034	6.449e-034	-33.118	-33.191	-0.073
Zn(OH)4-2	4.705e-034	2.382e-034	-33.327	-33.623	-0.296

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

Phase	SI	log IAP	log KT	
Al	-140.60	9.31	149.91	Al
Al(g)	-191.31	9.31	200.62	Al
Al2(SO4)3	-34.13	-15.23	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.78	-15.23	1.56	Al2(SO4)3:6H2O
Alum-K	-6.93	-11.90	-4.97	KAl(SO4)2:12H2O
Alunite	-1.38	-1.85	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.86	-5.21	-4.35	CaSO4
Antarcticite	-13.05	-8.95	4.09	CaCl2:6H2O
Antlerite	-9.76	-1.03	8.73	Cu3(SO4)(OH)4
Aphthitalite	-13.24	-17.13	-3.89	NaK3(SO4)2
Arcanite	-6.73	-8.57	-1.84	K2SO4
Arsenolite	-50.48	-70.32	-19.84	As2O3
As	-73.56	-30.87	42.68	As
As2O5	-17.11	-14.97	2.14	As2O5
As4O6(cubi)	-100.82	-140.64	-39.82	As4O6
As4O6(mono)	-100.59	-140.64	-40.05	As4O6
Atacamite	-16.57	-2.31	14.26	Cu4Cl2(OH)6
Bassanite	-1.50	-5.21	-3.71	CaSO4:0.5H2O
Birnessite	-10.64	-96.19	-85.55	Mn8O14:5H2O
Bischofite	-14.18	-9.79	4.39	MgCl2:6H2O
Bixbyite	-5.47	-6.43	-0.96	Mn2O3
Bloedite	-12.11	-14.59	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.52	5.03	7.55	AlO2H
Brochantite	-13.99	1.43	15.42	Cu4(SO4)(OH)6
Brucite	-13.90	2.38	16.28	Mg(OH)2
Ca	-133.76	6.07	139.83	Ca
Ca(g)	-159.00	6.07	165.07	Ca
Ca2Al2O5:8H2O	-43.09	16.48	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.03	-5.74	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-23.13	-5.32	17.80	Ca3(AsO4)2
Ca3Al2O6	-93.33	19.70	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-108.15	32.33	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-84.34	22.92	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-80.77	22.91	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-67.63	0.69	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-33.64	13.27	46.91	CaAl2O4
CaAl2O4:10H2O	-24.73	13.27	37.99	CaAl2O4:10H2O

CaAl4O7	-45.27	23.32	68.59	CaAl4O7
Carnallite	-20.21	-15.94	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.68	-5.21	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.33	-5.96	-2.63	CuSO4:5H2O
Chalcocyanite	-8.87	-5.96	2.91	CuSO4
Chloromagnesite	-31.60	-9.78	21.82	MgCl2
Cl2(g)	-18.02	-15.03	2.99	Cl2
Claudetite	-50.53	-70.32	-19.80	As2O3
Corundum	-8.24	10.05	18.29	Al2O3
Cu	-26.17	5.32	31.50	Cu
Cu(g)	-78.33	5.32	83.66	Cu
CuCl2	-13.42	-9.70	3.72	CuCl2
Cuprite	-27.83	-29.73	-1.91	Cu2O
Delafossite	-3.72	-10.16	-6.44	CuFeO2
Diaspore	-2.12	5.03	7.15	AlHO2
Epsomite	-4.08	-6.04	-1.96	MgSO4:7H2O
Ettringite	-58.40	4.06	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-58.50	0.51	59.02	Fe
Fe(OH)2	-16.24	-2.35	13.89	Fe(OH)2
Fe(OH)3	-0.93	4.71	5.64	Fe(OH)3
Fe2(SO4)3	-18.91	-15.87	3.05	Fe2(SO4)3
FeO	-15.87	-2.34	13.52	FeO
Ferrite-Ca	-8.87	12.63	21.50	CaFe2O4
Ferrite-Cu	1.60	11.88	10.28	CuFe2O4
Ferrite-Dicalcium	-40.95	15.85	56.80	Ca2Fe2O5
Ferrite-Mg	-9.22	11.80	21.02	MgFe2O4
Ferrite-Zn	-0.44	11.26	11.70	ZnFe2O4
FeSO4	-13.38	-10.77	2.61	FeSO4
Gibbsite	-2.71	5.03	7.74	Al(OH)3
Glauberite	-8.29	-13.75	-5.47	Na2Ca(SO4)2
Goethite	4.18	4.71	0.53	FeOOH
Gypsum	-0.68	-5.21	-4.53	CaSO4:2H2O
H2(g)	-40.14	-43.24	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.71	-6.14	1.56	NaCl
Hausmannite	-14.29	-4.14	10.14	Mn3O4
HCl(g)	-12.39	-6.08	6.30	HCl
Hematite	9.34	9.41	0.08	Fe2O3
Hercynite	-21.10	7.71	28.80	FeAl2O4
Hexahydrite	-4.32	-6.04	-1.73	MgSO4:6H2O
Hydrophilite	-20.70	-8.95	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	6.61	-2.81	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	2.66	-2.79	-5.45	NaFe3(SO4)2(OH)6
K	-69.62	1.36	70.98	K
K(g)	-80.22	1.36	81.58	K
K2O	-84.18	-0.14	84.04	K2O
K3H(SO4)2	-13.44	-17.07	-3.62	K3H(SO4)2
Kainite	-11.89	-12.20	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.17	-11.90	3.27	KAl(SO4)2
Katoite	-59.24	19.70	78.94	Ca3Al2H12O12
Kieserite	-5.78	-6.04	-0.27	MgSO4:H2O
KMgCl3	-37.19	-15.94	21.25	KMgCl3
KMgCl3:2H2O	-29.90	-15.94	13.96	KMgCl3:2H2O
Lammerite	-9.13	-7.58	1.55	Cu3(AsO4)2
Lawrencite	-23.57	-14.51	9.05	FeCl2
Leonite	-10.50	-14.61	-4.11	K2Mg(SO4)2:4H2O
Lime	-29.35	3.22	32.57	CaO
Magnetite	-3.35	7.07	10.42	Fe3O4
Manganite	-3.05	-3.22	-0.16	MnO(OH)
Manganosite	-15.63	2.29	17.92	MnO
Mayenite	-385.19	108.96	494.15	Ca12Al14O33
Melanterite	-8.37	-10.77	-2.40	FeSO4:7H2O
Mercallite	-7.06	-8.50	-1.44	KHSO4
Mg	-117.28	5.24	122.52	Mg
Mg(g)	-137.00	5.24	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.64	-5.45	5.20	Mg1.25SO4(OH)0.5:0.5H2O

Mg1.5SO4(OH)	-14.06	-4.85	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.52	-9.78	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.09	-9.79	7.30	MgCl2:4H2O
MgCl2:H2O	-25.86	-9.78	16.07	MgCl2:H2O
MgOHCl	-19.59	-3.70	15.89	MgOHCl
MgSO4	-10.87	-6.04	4.83	MgSO4
Mirabilite	-7.39	-8.55	-1.15	Na2SO4:10H2O
Misenite	-48.48	-59.56	-11.08	K8H6(SO4)7
Mn	-77.79	5.15	82.93	Mn
Mn(OH)2(am)	-13.02	2.29	15.31	Mn(OH)2
Mn(OH)3	-9.56	-3.22	6.34	Mn(OH)3
MnCl2:2H2O	-13.88	-9.88	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.63	-9.88	2.75	MnCl2:4H2O
MnCl2:H2O	-15.42	-9.88	5.54	MnCl2:H2O
MnO2(gamma)	-0.67	-16.79	-16.13	MnO2
MnSO4	-8.75	-6.14	2.61	MnSO4
Molysite	-27.02	-13.55	13.47	FeCl3
Na	-66.00	1.37	67.37	Na
Na(g)	-79.49	1.37	80.86	Na
Na2O	-67.53	-0.12	67.42	Na2O
Na3H(SO4)2	-16.14	-17.03	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.40	-22.30	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-15.24	4.65	19.88	NaFeO2
Nantokite	-14.18	-20.95	-6.77	CuCl
O2(g)	-2.82	-5.72	-2.89	O2
Oxychloride-Mg	-27.15	-1.32	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.66	-6.04	-1.39	MgSO4:5H2O
Periclase	-18.94	2.38	21.33	MgO
Picromerite	-10.17	-14.61	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-10.72	-25.03	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-19.33	3.22	22.55	Ca(OH)2
Pyrolusite	0.87	-16.79	-17.66	MnO2
Scacchite	-18.62	-9.88	8.74	MnCl2
Spinel	-25.17	12.44	37.61	Al2MgO4
Starkeyite	-5.04	-6.04	-1.00	MgSO4:4H2O
Sylvite	-6.98	-6.16	0.83	KCl
Syngenite	-6.18	-13.78	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-45.67	-28.52	17.14	Mg2CaCl6:12H2O
Tenorite	-5.18	2.47	7.65	CuO
Thenardite	-8.19	-8.54	-0.36	Na2SO4
Todorokite	-9.35	-55.17	-45.82	Mn7O12:3H2O
Wustite	-13.88	-1.47	12.40	Fe.947O
Zincite	-9.36	1.84	11.20	ZnO
Zn	-64.09	4.70	68.79	Zn
Zn(ClO4)2:6H2O	-70.27	-64.64	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.71	4.70	85.41	Zn
Zn(OH)2(beta)	-10.09	1.84	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.82	1.84	11.66	Zn(OH)2
Zn(OH)2(gamma)	-10.04	1.84	11.88	Zn(OH)2
Zn2(OH)3Cl	-17.69	-2.40	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-12.32	-4.74	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-18.76	-9.44	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-30.42	-11.33	19.09	Zn3O(SO4)2
ZnCl2	-17.40	-10.33	7.08	ZnCl2
ZnSO4	-10.12	-6.58	3.53	ZnSO4
ZnSO4:6H2O	-4.89	-6.58	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.71	-6.59	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.03	-6.58	-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
Hexahydrite	-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

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Beginning of batch-reaction calculations.  
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Reaction step 1.

Using mix 4.

Mixture 4.

1.000e+000 Solution 1 Flujo 3  
1.000e+000 Solution 4 AS3

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

Elements	Molality	Moles
Al	4.009e-004	8.019e-004
As	2.618e-005	5.236e-005
C	9.505e-004	1.901e-003
Ca	2.643e-003	5.286e-003
Cl	9.194e-004	1.839e-003
Cu	3.233e-004	6.466e-004
Fe	3.722e-004	7.445e-004
K	4.877e-004	9.755e-004
Mg	6.093e-004	1.219e-003
Mn	2.228e-004	4.456e-004
Na	1.391e-003	2.782e-003
S	7.857e-003	1.571e-002
Zn	7.586e-005	1.517e-004

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

pH	=	4.106	Charge balance
pe	=	15.888	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	2.103e-002	
Mass of water (kg)	=	2.000e+000	
Total alkalinity (eq/kg)	=	-2.046e-004	
Total CO2 (mol/kg)	=	9.505e-004	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-1.050e-002	
Percent error, 100*(Cat- An )/(Cat+ An )	=	-23.29	
Iterations	=	20	
Total H	=	2.221055e+002	
Total O	=	1.111201e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	8.807e-005	7.830e-005	-4.055	-4.106	-0.051
OH-	1.421e-010	1.230e-010	-9.847	-9.910	-0.063
H2O	5.553e+001	9.997e-001	1.744	-0.000	0.000
Al	4.009e-004				
AlSO4+	1.978e-004	1.717e-004	-3.704	-3.765	-0.061
Al+3	1.356e-004	4.637e-005	-3.868	-4.334	-0.466

Al(SO <sub>4</sub> ) <sub>2</sub> -	5.555e-005	4.822e-005	-4.255	-4.317	-0.061
AlOH+2	1.162e-005	6.632e-006	-4.935	-5.178	-0.243
Al(OH) <sub>2</sub> +	2.265e-007	1.966e-007	-6.645	-6.706	-0.061
Al <sub>2</sub> (OH) <sub>2</sub> +4	6.217e-008	7.153e-009	-7.206	-8.146	-0.939
HALO <sub>2</sub>	3.654e-009	3.654e-009	-8.437	-8.437	0.000
Al <sub>3</sub> (OH) <sub>4</sub> +5	9.626e-010	3.490e-011	-9.017	-10.457	-1.441
AlO <sub>2</sub> -	1.842e-011	1.599e-011	-10.735	-10.796	-0.061
NaAlO <sub>2</sub>	3.596e-015	3.596e-015	-14.444	-14.444	0.000
Al <sub>13</sub> O <sub>4</sub> (OH) <sub>24</sub> +7	1.417e-021	2.122e-024	-20.849	-23.673	-2.824
As(-3)	0.000e+000				
AsH <sub>3</sub>	0.000e+000	0.000e+000	-151.921	-151.921	0.000
As(3)	1.842e-027				
HAsO <sub>2</sub>	9.829e-028	9.829e-028	-27.007	-27.007	0.000
As(OH) <sub>3</sub>	8.592e-028	8.592e-028	-27.066	-27.066	0.000
H <sub>2</sub> AsO <sub>3</sub> -	7.730e-033	6.710e-033	-32.112	-32.173	-0.061
AsO <sub>2</sub> -	7.391e-033	6.417e-033	-32.131	-32.193	-0.061
AsO <sub>2</sub> OH-2	1.483e-039	8.373e-040	-38.829	-39.077	-0.248
HAsS <sub>2</sub>	0.000e+000	0.000e+000	-279.600	-279.600	0.000
As(5)	2.618e-005				
H <sub>2</sub> AsO <sub>4</sub> -	2.579e-005	2.239e-005	-4.589	-4.650	-0.061
H <sub>3</sub> AsO <sub>4</sub>	3.088e-007	3.088e-007	-6.510	-6.510	0.000
HAsO <sub>4</sub> -2	8.405e-008	4.746e-008	-7.075	-7.324	-0.248
AsO <sub>4</sub> -3	5.640e-015	1.555e-015	-14.249	-14.808	-0.560
C(-2)	0.000e+000				
C <sub>2</sub> H <sub>4</sub>	0.000e+000	0.000e+000	-255.140	-255.140	0.000
C(-3)	0.000e+000				
C <sub>2</sub> H <sub>6</sub>	0.000e+000	0.000e+000	-226.242	-226.242	0.000
C(-4)	0.000e+000				
CH <sub>4</sub>	0.000e+000	0.000e+000	-141.444	-141.444	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-48.053	-48.053	0.000
C(4)	9.505e-004				
CO <sub>2</sub>	9.443e-004	9.492e-004	-3.025	-3.023	0.002
HCO <sub>3</sub> -	6.018e-006	5.225e-006	-5.221	-5.282	-0.061
CaHCO <sub>3</sub> +	8.467e-008	7.351e-008	-7.072	-7.134	-0.061
MgHCO <sub>3</sub> +	1.636e-008	1.420e-008	-7.786	-7.848	-0.061
FeCO <sub>3</sub> +	1.323e-008	1.149e-008	-7.878	-7.940	-0.061
NaHCO <sub>3</sub>	8.812e-009	8.812e-009	-8.055	-8.055	0.000
ZnHCO <sub>3</sub> +	4.785e-009	4.154e-009	-8.320	-8.382	-0.061
MnHCO <sub>3</sub> +	3.938e-009	3.419e-009	-8.405	-8.466	-0.061
CuCO <sub>3</sub>	3.609e-009	3.609e-009	-8.443	-8.443	0.000
MnCO <sub>3</sub>	8.907e-012	8.907e-012	-11.050	-11.050	0.000
CaCO <sub>3</sub>	8.145e-012	8.145e-012	-11.089	-11.089	0.000
CO <sub>3</sub> -2	5.184e-012	2.960e-012	-11.285	-11.529	-0.243
FeHCO <sub>3</sub> +	2.864e-012	2.486e-012	-11.543	-11.604	-0.061
ZnCO <sub>3</sub>	7.667e-013	7.667e-013	-12.115	-12.115	0.000
MgCO <sub>3</sub>	7.329e-013	7.329e-013	-12.135	-12.135	0.000
NaCO <sub>3</sub> -	1.407e-014	1.221e-014	-13.852	-13.913	-0.061
FeCO <sub>3</sub>	1.524e-016	1.524e-016	-15.817	-15.817	0.000
Cu(CO <sub>3</sub> ) <sub>2</sub> -2	3.370e-017	1.903e-017	-16.472	-16.721	-0.248
CuCO <sub>3</sub> (OH) <sub>2</sub> -2	8.857e-021	5.001e-021	-20.053	-20.301	-0.248
Ca	2.643e-003				
Ca+2	2.015e-003	1.187e-003	-2.696	-2.925	-0.230
CaSO <sub>4</sub>	6.276e-004	6.276e-004	-3.202	-3.202	0.000
CaCl+	2.297e-007	1.994e-007	-6.639	-6.700	-0.061
CaHCO <sub>3</sub> +	8.467e-008	7.351e-008	-7.072	-7.134	-0.061
CaCl <sub>2</sub>	1.859e-010	1.859e-010	-9.731	-9.731	0.000
CaCO <sub>3</sub>	8.145e-012	8.145e-012	-11.089	-11.089	0.000
CaOH+	2.467e-012	2.141e-012	-11.608	-11.669	-0.061
Cl(-1)	9.194e-004				
Cl-	9.183e-004	7.924e-004	-3.037	-3.101	-0.064
CuCl+	3.191e-007	2.770e-007	-6.496	-6.557	-0.061
CaCl+	2.297e-007	1.994e-007	-6.639	-6.700	-0.061
MnCl+	1.671e-007	1.450e-007	-6.777	-6.839	-0.061
MgCl+	1.668e-007	1.448e-007	-6.778	-6.839	-0.061
NaCl	1.642e-007	1.642e-007	-6.785	-6.785	0.000
ZnCl+	4.730e-008	4.106e-008	-7.325	-7.387	-0.061

HCl	1.394e-008	1.394e-008	-7.856	-7.856	0.000
KCl	1.088e-008	1.088e-008	-7.963	-7.963	0.000
CaCl2	1.859e-010	1.859e-010	-9.731	-9.731	0.000
FeCl+2	1.554e-010	8.874e-011	-9.809	-10.052	-0.243
CuCl2	1.156e-010	1.156e-010	-9.937	-9.937	0.000
FeCl2+	6.557e-011	5.693e-011	-10.183	-10.245	-0.061
ZnCl2	3.801e-011	3.801e-011	-10.420	-10.420	0.000
Zn(OH)Cl	8.965e-012	8.965e-012	-11.047	-11.047	0.000
FeCl+	6.030e-013	5.235e-013	-12.220	-12.281	-0.061
MnCl3-	2.292e-014	1.989e-014	-13.640	-13.701	-0.061
ZnCl3-	1.916e-014	1.663e-014	-13.718	-13.779	-0.061
ZnCl4-2	1.770e-016	9.992e-017	-15.752	-16.000	-0.248
FeCl2	2.226e-018	2.226e-018	-17.652	-17.652	0.000
CuCl2-	4.338e-019	3.766e-019	-18.363	-18.424	-0.061
FeCl4-	4.950e-020	4.298e-020	-19.305	-19.367	-0.061
CuCl3-2	3.394e-021	1.917e-021	-20.469	-20.717	-0.248
CuCl4-2	2.413e-021	1.362e-021	-20.617	-20.866	-0.248
FeCl4-2	7.154e-024	4.039e-024	-23.145	-23.394	-0.248
Cl(1)	1.747e-018				
HClO	1.746e-018	1.746e-018	-17.758	-17.758	0.000
ClO-	6.926e-022	6.013e-022	-21.160	-21.221	-0.061
Cl(3)	7.372e-033				
ClO2-	6.699e-033	5.815e-033	-32.174	-32.235	-0.061
HClO2	6.732e-034	6.732e-034	-33.172	-33.172	0.000
Cl(5)	4.624e-030				
ClO3-	4.624e-030	4.003e-030	-29.335	-29.398	-0.063
Cl(7)	1.589e-031				
ClO4-	1.589e-031	1.375e-031	-30.799	-30.862	-0.063
ZnClO4+	9.241e-035	8.022e-035	-34.034	-34.096	-0.061
Cu(1)	1.086e-017				
Cu+	1.043e-017	9.052e-018	-16.982	-17.043	-0.061
CuCl2-	4.338e-019	3.766e-019	-18.363	-18.424	-0.061
CuCl3-2	3.394e-021	1.917e-021	-20.469	-20.717	-0.248
Cu(2)	3.233e-004				
Cu+2	2.169e-004	1.278e-004	-3.664	-3.893	-0.230
CuSO4	1.059e-004	1.059e-004	-3.975	-3.975	0.000
CuCl+	3.191e-007	2.770e-007	-6.496	-6.557	-0.061
CuOH+	9.696e-008	8.417e-008	-7.013	-7.075	-0.061
CuCO3	3.609e-009	3.609e-009	-8.443	-8.443	0.000
CuCl2	1.156e-010	1.156e-010	-9.937	-9.937	0.000
Cu(CO3)2-2	3.370e-017	1.903e-017	-16.472	-16.721	-0.248
CuCO3(OH)2-2	8.857e-021	5.001e-021	-20.053	-20.301	-0.248
CuCl4-2	2.413e-021	1.362e-021	-20.617	-20.866	-0.248
CuO2-2	2.137e-027	1.206e-027	-26.670	-26.918	-0.248
Fe(2)	2.063e-009				
Fe+2	1.539e-009	9.068e-010	-8.813	-9.042	-0.230
FeSO4	5.201e-010	5.201e-010	-9.284	-9.284	0.000
FeHCO3+	2.864e-012	2.486e-012	-11.543	-11.604	-0.061
FeCl+	6.030e-013	5.235e-013	-12.220	-12.281	-0.061
FeOH+	4.217e-015	3.661e-015	-14.375	-14.436	-0.061
FeCO3	1.524e-016	1.524e-016	-15.817	-15.817	0.000
FeCl2	2.226e-018	2.226e-018	-17.652	-17.652	0.000
Fe(OH)2	3.713e-022	3.713e-022	-21.430	-21.430	0.000
FeCl4-2	7.154e-024	4.039e-024	-23.145	-23.394	-0.248
Fe(OH)3-	2.174e-028	1.887e-028	-27.663	-27.724	-0.061
Fe(OH)4-2	4.268e-039	2.410e-039	-38.370	-38.618	-0.248
Fe(3)	3.722e-004				
Fe(OH)2+	2.698e-004	2.342e-004	-3.569	-3.630	-0.061
FeOH+2	9.702e-005	5.540e-005	-4.013	-4.256	-0.243
Fe+3	1.966e-006	6.720e-007	-5.706	-6.173	-0.466
Fe(OH)3	1.399e-006	1.399e-006	-5.854	-5.854	0.000
Fe2(OH)2+4	7.180e-007	8.260e-008	-6.144	-7.083	-0.939
FeSO4+	2.710e-007	2.353e-007	-6.567	-6.628	-0.061
Fe3(OH)4+5	1.115e-007	4.042e-009	-6.953	-8.393	-1.441
Fe(SO4)2-	1.658e-008	1.439e-008	-7.780	-7.842	-0.061
FeCO3+	1.323e-008	1.149e-008	-7.878	-7.940	-0.061
FeCl+2	1.554e-010	8.874e-011	-9.809	-10.052	-0.243

FeCl2+	6.557e-011	5.693e-011	-10.183	-10.245	-0.061
Fe(OH)4-	5.167e-012	4.486e-012	-11.287	-11.348	-0.061
FeCl4-	4.950e-020	4.298e-020	-19.305	-19.367	-0.061
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.091	-43.089	0.002
K	4.877e-004				
K+	4.740e-004	4.090e-004	-3.324	-3.388	-0.064
KSO4-	1.376e-005	1.195e-005	-4.861	-4.923	-0.061
KCl	1.088e-008	1.088e-008	-7.963	-7.963	0.000
KHSO4	8.253e-010	8.253e-010	-9.083	-9.083	0.000
KOH	1.811e-014	1.811e-014	-13.742	-13.742	0.000
Mg	6.093e-004				
Mg+2	3.830e-004	2.341e-004	-3.417	-3.631	-0.214
MgSO4	2.262e-004	2.262e-004	-3.646	-3.646	0.000
MgCl+	1.668e-007	1.448e-007	-6.778	-6.839	-0.061
MgHCO3+	1.636e-008	1.420e-008	-7.786	-7.848	-0.061
MgCO3	7.329e-013	7.329e-013	-12.135	-12.135	0.000
Mg4(OH)4+4	1.233e-037	1.418e-038	-36.909	-37.848	-0.939
Mn(2)	2.228e-004				
Mn+2	1.459e-004	8.595e-005	-3.836	-4.066	-0.230
MnSO4	7.674e-005	7.674e-005	-4.115	-4.115	0.000
MnCl+	1.671e-007	1.450e-007	-6.777	-6.839	-0.061
MnHCO3+	3.938e-009	3.419e-009	-8.405	-8.466	-0.061
MnOH+	3.249e-011	2.821e-011	-10.488	-10.550	-0.061
MnCO3	8.907e-012	8.907e-012	-11.050	-11.050	0.000
MnCl3-	2.292e-014	1.989e-014	-13.640	-13.701	-0.061
Mn2OH+3	8.968e-015	2.598e-015	-14.047	-14.585	-0.538
Mn(OH)2	8.840e-019	8.840e-019	-18.054	-18.054	0.000
Mn2(OH)3+	2.230e-020	1.936e-020	-19.652	-19.713	-0.061
Mn(OH)3-	1.220e-026	1.059e-026	-25.914	-25.975	-0.061
Mn(OH)4-2	2.027e-036	1.145e-036	-35.693	-35.941	-0.248
Mn(3)	6.117e-014				
Mn+3	6.117e-014	1.772e-014	-13.213	-13.752	-0.538
Mn(6)	1.372e-026				
MnO4-2	1.372e-026	7.749e-027	-25.863	-26.111	-0.248
Mn(7)	3.047e-020				
MnO4-	3.047e-020	2.637e-020	-19.516	-19.579	-0.063
Na	1.391e-003				
Na+	1.358e-003	1.179e-003	-2.867	-2.928	-0.061
NaSO4-	3.247e-005	2.819e-005	-4.488	-4.550	-0.061
NaCl	1.642e-007	1.642e-007	-6.785	-6.785	0.000
NaHCO3	8.812e-009	8.812e-009	-8.055	-8.055	0.000
NaOH	2.503e-014	2.503e-014	-13.602	-13.602	0.000
NaCO3-	1.407e-014	1.221e-014	-13.852	-13.913	-0.061
NaAlO2	3.596e-015	3.596e-015	-14.444	-14.444	0.000
O(0)	1.910e-006				
O2	9.548e-007	9.597e-007	-6.020	-6.018	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-129.891	-129.891	0.000
HS-	0.000e+000	0.000e+000	-132.732	-132.795	-0.063
S-2	0.000e+000	0.000e+000	-141.376	-141.614	-0.239
S2-2	0.000e+000	0.000e+000	-235.092	-235.340	-0.248
HAsS2	0.000e+000	0.000e+000	-279.600	-279.600	0.000
S3-2	0.000e+000	0.000e+000	-328.859	-329.108	-0.248
S4-2	0.000e+000	0.000e+000	-422.854	-423.102	-0.248
S5-2	0.000e+000	0.000e+000	-517.065	-517.313	-0.248
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-134.285	-134.533	-0.248
HS2O3-	0.000e+000	0.000e+000	-137.564	-137.626	-0.061
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-122.232	-122.471	-0.239
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-42.864	-42.925	-0.061
H2SO3	0.000e+000	0.000e+000	-45.050	-45.050	0.000
SO2	0.000e+000	0.000e+000	-45.150	-45.150	0.000
SO3-2	0.000e+000	0.000e+000	-45.807	-46.050	-0.243
S2O6-2	0.000e+000	0.000e+000	-61.207	-61.455	-0.248



S306-2	0.000e+000	0.000e+000	-157.457	-157.705	-0.248
S406-2	0.000e+000	0.000e+000	-237.801	-238.050	-0.248
S506-2	0.000e+000	0.000e+000	-347.025	-347.274	-0.248
S(5)	0.000e+000				
S205-2	0.000e+000	0.000e+000	-90.432	-90.680	-0.248
S(6)	7.857e-003				
SO4-2	6.409e-003	3.618e-003	-2.193	-2.441	-0.248
CaSO4	6.276e-004	6.276e-004	-3.202	-3.202	0.000
MgSO4	2.262e-004	2.262e-004	-3.646	-3.646	0.000
AlSO4+	1.978e-004	1.717e-004	-3.704	-3.765	-0.061
CuSO4	1.059e-004	1.059e-004	-3.975	-3.975	0.000
MnSO4	7.674e-005	7.674e-005	-4.115	-4.115	0.000
Al(SO4)2-	5.555e-005	4.822e-005	-4.255	-4.317	-0.061
HSO4-	3.297e-005	2.862e-005	-4.482	-4.543	-0.061
NaSO4-	3.247e-005	2.819e-005	-4.488	-4.550	-0.061
ZnSO4	2.345e-005	2.345e-005	-4.630	-4.630	0.000
KSO4-	1.376e-005	1.195e-005	-4.861	-4.923	-0.061
FeSO4+	2.710e-007	2.353e-007	-6.567	-6.628	-0.061
Fe(SO4)2-	1.658e-008	1.439e-008	-7.780	-7.842	-0.061
KHSO4	8.253e-010	8.253e-010	-9.083	-9.083	0.000
FeSO4	5.201e-010	5.201e-010	-9.284	-9.284	0.000
H2SO4	2.114e-012	2.114e-012	-11.675	-11.675	0.000
S(7)	9.772e-039				
S208-2	4.886e-039	2.759e-039	-38.311	-38.559	-0.248
S(8)	1.754e-027				
HSO5-	1.754e-027	1.523e-027	-26.756	-26.817	-0.061
Zn	7.586e-005				
Zn+2	5.236e-005	3.084e-005	-4.281	-4.511	-0.230
ZnSO4	2.345e-005	2.345e-005	-4.630	-4.630	0.000
ZnCl+	4.730e-008	4.106e-008	-7.325	-7.387	-0.061
ZnHCO3+	4.785e-009	4.154e-009	-8.320	-8.382	-0.061
ZnOH+	4.975e-010	4.319e-010	-9.303	-9.365	-0.061
ZnCl2	3.801e-011	3.801e-011	-10.420	-10.420	0.000
Zn(OH)Cl	8.965e-012	8.965e-012	-11.047	-11.047	0.000
ZnCO3	7.667e-013	7.667e-013	-12.115	-12.115	0.000
Zn(OH)2	2.362e-014	2.362e-014	-13.627	-13.627	0.000
ZnCl3-	1.916e-014	1.663e-014	-13.718	-13.779	-0.061
ZnCl4-2	1.770e-016	9.992e-017	-15.752	-16.000	-0.248
Zn(OH)3-	1.077e-021	9.346e-022	-20.968	-21.029	-0.061
Zn(OH)4-2	3.603e-030	2.034e-030	-29.443	-29.692	-0.248
ZnClO4+	9.241e-035	8.022e-035	-34.034	-34.096	-0.061

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

Phase	SI	log IAP	log KT	
Al	-137.42	12.50	149.91	Al
Al(g)	-188.12	12.50	200.62	Al
Al2(SO4)3	-34.89	-15.99	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-17.55	-15.99	1.56	Al2(SO4)3:6H2O
Alabandite	-132.33	-132.75	-0.42	MnS
Alum-K	-7.64	-12.61	-4.97	KAl(SO4)2:12H2O
Alunite	3.83	3.36	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.02	-5.37	-4.35	CaSO4
Antarcticite	-13.22	-9.13	4.09	CaCl2:6H2O
Antlerite	-6.43	2.30	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.09	-17.98	-3.89	NaK3(SO4)2
Aragonite	-6.07	-4.10	1.97	CaCO3
Arcanite	-7.37	-9.22	-1.84	K2SO4
Arsenolite	-52.72	-72.56	-19.84	As2O3
Arsenopyrite	-217.39	-231.83	-14.45	FeAsS
Artinite	-19.85	-0.23	19.63	Mg2CO3(OH)2:3H2O
As	-74.45	-31.77	42.68	As
As2O5	-19.65	-17.51	2.14	As2O5
As4O6(cubi)	-105.29	-145.12	-39.82	As4O6
As4O6(mono)	-105.07	-145.12	-40.05	As4O6
Atacamite	-11.40	2.86	14.26	Cu4Cl2(OH)6

Azurite	-14.94	-5.82	9.12	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$
Bassanite	-1.66	-5.37	-3.71	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
Birnessite	3.31	-82.24	-85.55	$\text{Mn}_8\text{O}_{14} \cdot 5\text{H}_2\text{O}$
Bischofite	-14.23	-9.83	4.39	$\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$
Bixbyite	-1.90	-2.87	-0.96	$\text{Mn}_2\text{O}_3$
Bloedite	-11.89	-14.37	-2.48	$\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$
Boehmite	0.44	7.98	7.55	$\text{AlO}_2\text{H}$
Bornite	-493.33	-595.86	-102.53	$\text{Cu}_5\text{FeS}_4$
Brochantite	-8.80	6.62	15.42	$\text{Cu}_4(\text{SO}_4)(\text{OH})_6$
Brucite	-11.70	4.58	16.28	$\text{Mg}(\text{OH})_2$
Burkeite	-33.12	-23.63	9.49	$\text{Na}_6\text{CO}_3(\text{SO}_4)_2$
C	-67.52	-3.37	64.15	C
C(g)	-185.14	-3.37	181.77	C
Ca	-131.54	8.30	139.83	Ca
Ca(g)	-156.78	8.30	165.07	Ca
$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$	-33.03	26.54	59.57	$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$
$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$	-30.13	-3.84	26.29	$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$
$\text{Ca}_3(\text{AsO}_4)_2$	-19.45	-1.65	17.80	$\text{Ca}_3(\text{AsO}_4)_2$
$\text{Ca}_3\text{Al}_2\text{O}_6$	-81.20	31.83	113.03	$\text{Ca}_3\text{Al}_2\text{O}_6$
$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$	-91.07	49.41	140.48	$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$	-70.14	37.12	107.25	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$	-66.57	37.11	103.68	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$
$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$	-61.60	6.73	68.33	$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$
$\text{CaAl}_2\text{O}_4$	-25.65	21.26	46.91	$\text{CaAl}_2\text{O}_4$
$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$	-16.74	21.26	37.99	$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$
$\text{CaAl}_4\text{O}_7$	-31.37	37.23	68.59	$\text{CaAl}_4\text{O}_7$
Calcite	-5.93	-4.10	1.82	$\text{CaCO}_3$
Carnallite	-20.59	-16.32	4.27	$\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$
$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}(\text{beta})$	-1.83	-5.37	-3.54	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
$\text{CH}_4(\text{g})$	-138.60	-141.44	-2.84	$\text{CH}_4$
Chalcanthite	-3.71	-6.34	-2.63	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
Chalcocite	-128.03	-162.77	-34.74	$\text{Cu}_2\text{S}$
Chalcocyanite	-9.25	-6.33	2.91	$\text{CuSO}_4$
Chalcopyrite	-237.71	-270.31	-32.60	$\text{CuFeS}_2$
Chloromagnesite	-31.65	-9.83	21.82	$\text{MgCl}_2$
$\text{Cl}_2(\text{g})$	-20.42	-17.42	2.99	$\text{Cl}_2$
Claudetite	-52.76	-72.56	-19.80	$\text{As}_2\text{O}_3$
$\text{CO}(\text{g})$	-45.06	-48.05	-3.00	CO
$\text{CO}_2(\text{g})$	-1.56	-9.39	-7.83	$\text{CO}_2$
Corundum	-2.32	15.97	18.29	$\text{Al}_2\text{O}_3$
Covellite	-109.72	-132.58	-22.86	CuS
Cu	-24.17	7.33	31.50	Cu
Cu(g)	-76.33	7.33	83.66	Cu
$\text{CuCl}_2$	-13.82	-10.10	3.72	$\text{CuCl}_2$
Cuprite	-23.97	-25.87	-1.91	$\text{Cu}_2\text{O}$
Dawsonite	-4.57	-0.23	4.34	$\text{NaAlCO}_3(\text{OH})_2$
Delafossite	-0.36	-6.79	-6.44	$\text{CuFeO}_2$
Diaspore	0.84	7.98	7.15	$\text{AlHO}_2$
Dolomite	-11.38	-8.91	2.47	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-dis	-12.92	-8.91	4.01	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-ord	-11.37	-8.91	2.46	$\text{CaMg}(\text{CO}_3)_2$
Epsomite	-4.11	-6.07	-1.96	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$
Ettringite	-46.74	15.73	62.46	$\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O}$
Fe	-56.84	2.18	59.02	Fe
$\text{Fe}(\text{OH})_2$	-14.72	-0.83	13.89	$\text{Fe}(\text{OH})_2$
$\text{Fe}(\text{OH})_3$	0.51	6.15	5.64	$\text{Fe}(\text{OH})_3$
$\text{Fe}_2(\text{SO}_4)_3$	-22.72	-19.67	3.05	$\text{Fe}_2(\text{SO}_4)_3$
FeO	-14.35	-0.83	13.52	FeO
Ferrite-Ca	-3.92	17.58	21.50	$\text{CaFe}_2\text{O}_4$
Ferrite-Cu	6.33	16.61	10.28	$\text{CuFe}_2\text{O}_4$
Ferrite-Dicalcium	-33.93	22.87	56.80	$\text{Ca}_2\text{Fe}_2\text{O}_5$
Ferrite-Mg	-4.15	16.87	21.02	$\text{MgFe}_2\text{O}_4$
Ferrite-Zn	4.29	15.99	11.70	$\text{ZnFe}_2\text{O}_4$
$\text{FeSO}_4$	-14.09	-11.48	2.61	$\text{FeSO}_4$
Gaylussite	-22.30	-11.13	11.16	$\text{CaNa}_2(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$
Gibbsite	0.24	7.98	7.74	$\text{Al}(\text{OH})_3$
Glauberite	-8.20	-13.67	-5.47	$\text{Na}_2\text{Ca}(\text{SO}_4)_2$

Goethite	5.62	6.15	0.53	FeOOH
Gypsum	-0.84	-5.37	-4.53	CaSO4:2H2O
H2(g)	-39.99	-43.09	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-128.91	-136.90	-7.99	H2S
Halite	-7.59	-6.03	1.56	NaCl
Hausmannite	-8.86	1.28	10.14	Mn3O4
HCl(g)	-13.51	-7.21	6.30	HCl
Hematite	12.22	12.29	0.08	Fe2O3
Hercynite	-13.66	15.14	28.80	FeAl2O4
Hexahydrite	-4.35	-6.07	-1.73	MgSO4:6H2O
Huntite	-28.74	-18.52	10.22	CaMg3(CO3)4
Hydromagnesite	-45.38	-14.64	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.87	-9.13	11.75	CaCl2
Hydrozincite	-30.58	-0.27	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.26	-2.15	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.76	-1.69	-5.45	NaFe3(SO4)2(OH)6
K	-68.75	2.22	70.98	K
K(g)	-79.36	2.22	81.58	K
K2CO3:1.5H2O	-21.33	-7.95	13.38	K2CO3:1.5H2O
K2O	-82.60	1.44	84.04	K2O
K3H(SO4)2	-15.53	-19.15	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-78.30	-50.59	27.71	K8H4(CO3)6:3H2O
Kainite	-12.25	-12.56	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.88	-12.61	3.27	KAl(SO4)2
Kaliginite	-8.95	-8.67	0.28	KHCO3
Katoite	-47.11	31.83	78.94	Ca3Al2H12O12
Kieserite	-5.81	-6.07	-0.27	MgSO4:H2O
KMgCl3	-37.57	-16.32	21.25	KMgCl3
KMgCl3:2H2O	-30.28	-16.32	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-17.75	-7.49	10.26	KNaCO3:6H2O
Lammerite	-6.11	-4.56	1.55	Cu3(AsO4)2
Lansfordite	-9.65	-4.81	4.84	MgCO3:5H2O
Lawrencite	-24.30	-15.24	9.05	FeCl2
Leonite	-11.18	-15.29	-4.11	K2Mg(SO4)2:4H2O
Lime	-27.28	5.29	32.57	CaO
Magnesite	-7.08	-4.81	2.27	MgCO3
Magnetite	1.04	11.46	10.42	Fe3O4
Malachite	-6.65	-0.75	5.90	Cu2CO3(OH)2
Manganite	-1.27	-1.43	-0.16	MnO(OH)
Manganosite	-13.77	4.15	17.92	MnO
Mayenite	-318.92	175.23	494.15	Ca12Al14O33
Melanterite	-9.09	-11.48	-2.40	FeSO4:7H2O
Mercallite	-8.50	-9.94	-1.44	KHSO4
Mg	-114.93	7.59	122.52	Mg
Mg(g)	-134.65	7.59	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.12	-4.93	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-12.99	-3.78	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.56	-9.83	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.13	-9.83	7.30	MgCl2:4H2O
MgCl2:H2O	-25.90	-9.83	16.07	MgCl2:H2O
MgOHCl	-18.52	-2.63	15.89	MgOHCl
MgSO4	-10.90	-6.07	4.83	MgSO4
Mirabilite	-7.15	-8.30	-1.15	Na2SO4:10H2O
Misenite	-57.76	-68.83	-11.08	K8H6(SO4)7
Mn	-75.78	7.16	82.93	Mn
Mn(OH)2(am)	-11.16	4.15	15.31	Mn(OH)2
Mn(OH)3	-7.77	-1.43	6.34	Mn(OH)3
MnCl2:2H2O	-14.27	-10.27	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.02	-10.27	2.75	MnCl2:4H2O
MnCl2:H2O	-15.81	-10.27	5.54	MnCl2:H2O
MnO2(gamma)	1.04	-15.09	-16.13	MnO2
MnSO4	-9.12	-6.51	2.61	MnSO4
Molysite	-28.95	-15.48	13.47	FeCl3
Monohydrocalcite	-6.78	-4.10	2.68	CaCO3:H2O
Na	-64.69	2.68	67.37	Na

Na(g)	-78.18	2.68	80.86	Na
Na2CO3	-18.20	-7.03	11.16	Na2CO3
Na2CO3:7H2O	-16.97	-7.03	9.94	Na2CO3:7H2O
Na2O	-65.06	2.36	67.42	Na2O
Na3H(SO4)2	-16.88	-17.77	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.07	-21.96	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-12.56	7.32	19.88	NaFeO2
Nahcolite	-8.07	-8.21	-0.14	NaHCO3
Nantokite	-13.38	-20.14	-6.77	CuCl
Natron	-16.62	-7.03	9.59	Na2CO3:10H2O
Nesquehonite	-10.10	-4.81	5.29	MgCO3:3H2O
O2(g)	-3.13	-6.02	-2.89	O2
Orpiment	-403.78	-483.26	-79.49	As2S3
Oxychloride-Mg	-23.88	1.96	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.69	-6.07	-1.39	MgSO4:5H2O
Periclase	-16.74	4.58	21.33	MgO
Picromerite	-10.85	-15.29	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-22.46	-11.13	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-11.71	-26.02	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-17.26	5.29	22.55	Ca(OH)2
Pyrite	-218.37	-243.07	-24.70	FeS2
Pyrolusite	2.57	-15.09	-17.66	MnO2
Pyrrhotite	-133.99	-137.73	-3.74	FeS
Realgar	-156.99	-217.26	-60.28	AsS
Rhodochrosite	-5.02	-5.24	-0.22	MnCO3
S	-94.80	-139.91	-45.11	S
S2(g)	-203.49	-210.68	-7.19	S2
Scacchite	-19.01	-10.27	8.74	MnCl2
Siderite	-10.00	-10.22	-0.22	FeCO3
Smithsonite	-6.13	-5.69	0.44	ZnCO3
SO2(g)	-45.33	-45.15	0.18	SO2
Sphalerite	-121.73	-133.20	-11.47	ZnS
Spinel	-17.05	20.55	37.61	Al2MgO4
Starkeyite	-5.07	-6.07	-1.00	MgSO4:4H2O
Sylvite	-7.32	-6.49	0.83	KCl
Syngenite	-6.98	-14.59	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.94	-28.79	17.14	Mg2CaCl6:12H2O
Tenorite	-3.33	4.32	7.65	CuO
Thenardite	-7.94	-8.30	-0.36	Na2SO4
Thermonatrite	-17.97	-7.03	10.94	Na2CO3:H2O
Todorokite	2.90	-42.92	-45.82	Mn7O12:3H2O
Troilite	-133.89	-137.73	-3.84	FeS
Trona-K	-27.75	-16.16	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-124.03	-133.20	-9.17	ZnS
Wustite	-12.45	-0.05	12.40	Fe.947O
Zincite	-7.50	3.70	11.20	ZnO
Zn	-62.08	6.71	68.79	Zn
Zn(ClO4)2:6H2O	-71.87	-66.23	5.63	Zn(ClO4)2:6H2O
Zn(g)	-78.70	6.71	85.41	Zn
Zn(OH)2(beta)	-8.23	3.70	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-7.96	3.70	11.66	Zn(OH)2
Zn(OH)2(gamma)	-8.18	3.70	11.88	Zn(OH)2
Zn2(OH)3Cl	-15.10	0.20	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-10.83	-3.25	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-15.72	-6.41	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-29.29	-10.20	19.09	Zn3O(SO4)2
ZnCl2	-17.79	-10.71	7.08	ZnCl2
ZnCO3:H2O	-5.83	-5.69	0.14	ZnCO3:H2O
ZnSO4	-10.49	-6.95	3.53	ZnSO4
ZnSO4:6H2O	-5.25	-6.95	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.08	-6.95	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.40	-6.95	-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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