
Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat
SOLUTION 1 UGA1

temp	25
pH	4.44
pe	12
redox	pe
units	mg/l
density	1
Cl	51.73
S(6)	261.82
Al	1.14
As	0.01
Ca	35.55
Cu	0.13
Fe	5.48
K	25.35
Mg	3.69
Mn	5.09
Na	18.1
Zn	0.56
C(4)	0
N(5)	50.06
water	1 # kg

SOLUTION 2 UGA2

temp	25
pH	2.46
pe	12
redox	pe
units	mg/l
density	1
Cl	35.56
S(6)	1972
Al	19.29
As	0.68
Ca	33.94
Cu	0.024
Fe	100
K	1.44
Mg	23.2
Mn	7.37
Na	8.26
Zn	2.8

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C(4)      1.22
N(5)      48.65
water     1 # kg
MIX 1
  1      6
  2      4
SELECTED_OUTPUT
file      MISDAMFLUJO2
ph        true
totals    Al As Cu Fe Mg Mn Zn
          S

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Beginning of initial solution calculations.

Initial solution 1. UGA1

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

Elements	Molality	Moles
Al	4.227e-005	4.227e-005
As	1.335e-007	1.335e-007
Ca	8.874e-004	8.874e-004
Cl	1.460e-003	1.460e-003
Cu	2.047e-006	2.047e-006
Fe	9.817e-005	9.817e-005
K	6.487e-004	6.487e-004
Mg	1.519e-004	1.519e-004
Mn	9.269e-005	9.269e-005
N(5)	3.576e-003	3.576e-003
Na	7.877e-004	7.877e-004
S(6)	2.727e-003	2.727e-003
Zn	8.568e-006	8.568e-006

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

```

pH = 4.440
pe = 12.000
Activity of water = 1.000
Ionic strength = 1.035e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -5.383e-005
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -6.489e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -47.60
Iterations = 4
Total H = 1.110509e+002
Total O = 5.554715e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.977e-005	3.631e-005	-4.400	-4.440	-0.040
OH-	2.951e-010	2.653e-010	-9.530	-9.576	-0.046
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	4.227e-005				
Al+3	1.980e-005	8.654e-006	-4.703	-5.063	-0.359
AlSO4+	1.615e-005	1.455e-005	-4.792	-4.837	-0.045
AlOH+2	4.045e-006	2.670e-006	-5.393	-5.574	-0.180
Al(SO4)2-	2.060e-006	1.855e-006	-5.686	-5.732	-0.045
Al(OH)2+	1.896e-007	1.707e-007	-6.722	-6.768	-0.045
HALO2	6.843e-009	6.843e-009	-8.165	-8.165	0.000

Al2(OH)2+4	5.845e-009	1.159e-009	-8.233	-8.936	-0.703
AlO2-	7.169e-011	6.456e-011	-10.145	-10.190	-0.045
Al3(OH)4+5	5.943e-011	4.910e-012	-10.226	-11.309	-1.083
NaAlO2	8.641e-015	8.641e-015	-14.063	-14.063	0.000
Al13O4(OH)24+7	4.516e-021	3.403e-023	-20.345	-22.468	-2.123
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-126.095	-126.095	0.000
As(3)	5.823e-023				
HAsO2	3.107e-023	3.107e-023	-22.508	-22.508	0.000
As(OH)3	2.716e-023	2.716e-023	-22.566	-22.566	0.000
H2AsO3-	5.080e-028	4.575e-028	-27.294	-27.340	-0.045
AsO2-	4.857e-028	4.374e-028	-27.314	-27.359	-0.045
AsO2OH-2	1.877e-034	1.231e-034	-33.727	-33.910	-0.183
As(5)	1.335e-007				
H2AsO4-	1.319e-007	1.188e-007	-6.880	-6.925	-0.045
HAsO4-2	8.283e-010	5.433e-010	-9.082	-9.265	-0.183
H3AsO4	7.600e-010	7.600e-010	-9.119	-9.119	0.000
AsO4-3	9.926e-017	3.839e-017	-16.003	-16.416	-0.413
Ca	8.874e-004				
Ca+2	7.563e-004	5.079e-004	-3.121	-3.294	-0.173
CaSO4	1.219e-004	1.219e-004	-3.914	-3.914	0.000
CaNO3+	9.050e-006	8.150e-006	-5.043	-5.089	-0.045
CaCl+	1.566e-007	1.410e-007	-6.805	-6.851	-0.045
CaCl2	2.173e-010	2.173e-010	-9.663	-9.663	0.000
CaOH+	2.194e-012	1.976e-012	-11.659	-11.704	-0.045
Cl(-1)	1.460e-003				
Cl-	1.459e-003	1.310e-003	-2.836	-2.883	-0.047
NaCl	1.615e-007	1.615e-007	-6.792	-6.792	0.000
CaCl+	1.566e-007	1.410e-007	-6.805	-6.851	-0.045
MnCl+	1.508e-007	1.358e-007	-6.821	-6.867	-0.045
MgCl+	9.088e-008	8.185e-008	-7.042	-7.087	-0.045
KCl	2.528e-008	2.528e-008	-7.597	-7.597	0.000
ZnCl+	1.140e-008	1.027e-008	-7.943	-7.989	-0.045
HCl	1.068e-008	1.068e-008	-7.971	-7.971	0.000
CuCl+	4.352e-009	3.920e-009	-8.361	-8.407	-0.045
FeCl+	5.138e-010	4.627e-010	-9.289	-9.335	-0.045
CaCl2	2.173e-010	2.173e-010	-9.663	-9.663	0.000
ZnCl2	1.571e-011	1.571e-011	-10.804	-10.804	0.000
FeCl+2	1.538e-011	1.015e-011	-10.813	-10.994	-0.180
FeCl2+	1.195e-011	1.076e-011	-10.923	-10.968	-0.045
Zn(OH)Cl	4.834e-012	4.834e-012	-11.316	-11.316	0.000
CuCl2	2.704e-012	2.704e-012	-11.568	-11.568	0.000
MnCl3-	5.654e-014	5.092e-014	-13.248	-13.293	-0.045
ZnCl3-	1.262e-014	1.136e-014	-13.899	-13.944	-0.045
FeCl2	3.253e-015	3.253e-015	-14.488	-14.488	0.000
ZnCl4-2	1.720e-016	1.128e-016	-15.764	-15.948	-0.183
CuCl2-	7.559e-017	6.808e-017	-16.122	-16.167	-0.045
CuCl3-2	8.732e-019	5.727e-019	-18.059	-18.242	-0.183
FeCl4-	2.465e-020	2.220e-020	-19.608	-19.654	-0.045
FeCl4-2	2.459e-020	1.613e-020	-19.609	-19.792	-0.183
CuCl4-2	1.327e-022	8.707e-023	-21.877	-22.060	-0.183
Cl(1)	1.043e-025				
HClO	1.042e-025	1.042e-025	-24.982	-24.982	0.000
ClO-	8.593e-029	7.739e-029	-28.066	-28.111	-0.045
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-46.189	-46.234	-0.045
HClO2	0.000e+000	0.000e+000	-47.505	-47.505	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-50.459	-50.505	-0.046
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-59.032	-59.078	-0.046
ZnClO4+	0.000e+000	0.000e+000	-63.087	-63.133	-0.045
Cu(1)	7.414e-016				
Cu+	6.649e-016	5.988e-016	-15.177	-15.223	-0.045
CuCl2-	7.559e-017	6.808e-017	-16.122	-16.167	-0.045
CuCl3-2	8.732e-019	5.727e-019	-18.059	-18.242	-0.183
Cu(2)	2.047e-006				

Cu+2	1.629e-006	1.094e-006	-5.788	-5.961	-0.173
CuSO4	4.117e-007	4.117e-007	-6.385	-6.385	0.000
CuCl+	4.352e-009	3.920e-009	-8.361	-8.407	-0.045
CuOH+	1.725e-009	1.554e-009	-8.763	-8.809	-0.045
CuCl2	2.704e-012	2.704e-012	-11.568	-11.568	0.000
CuCl4-2	1.327e-022	8.707e-023	-21.877	-22.060	-0.183
CuO2-2	3.406e-028	2.234e-028	-27.468	-27.651	-0.183
Fe(2)	8.488e-007				
Fe+2	7.220e-007	4.849e-007	-6.141	-6.314	-0.173
FeSO4	1.262e-007	1.262e-007	-6.899	-6.899	0.000
FeCl+	5.138e-010	4.627e-010	-9.289	-9.335	-0.045
FeOH+	4.688e-012	4.222e-012	-11.329	-11.374	-0.045
FeCl2	3.253e-015	3.253e-015	-14.488	-14.488	0.000
Fe(OH)2	9.236e-019	9.236e-019	-18.035	-18.035	0.000
FeCl4-2	2.459e-020	1.613e-020	-19.609	-19.792	-0.183
Fe(OH)3-	1.124e-024	1.013e-024	-23.949	-23.995	-0.045
Fe(OH)4-2	4.251e-035	2.788e-035	-34.372	-34.555	-0.183
Fe(3)	9.732e-005				
Fe(OH)2+	8.369e-005	7.537e-005	-4.077	-4.123	-0.045
FeOH+2	1.252e-005	8.266e-006	-4.902	-5.083	-0.180
Fe(OH)3	9.708e-007	9.708e-007	-6.013	-6.013	0.000
Fe+3	1.064e-007	4.649e-008	-6.973	-7.333	-0.359
Fe2(OH)2+4	9.274e-009	1.839e-009	-8.033	-8.735	-0.703
FeSO4+	8.205e-009	7.389e-009	-8.086	-8.131	-0.045
FeNO3+2	2.255e-009	1.488e-009	-8.647	-8.827	-0.180
Fe3(OH)4+5	3.505e-010	2.896e-011	-9.455	-10.538	-1.083
Fe(SO4)2-	2.279e-010	2.052e-010	-9.642	-9.688	-0.045
FeCl+2	1.538e-011	1.015e-011	-10.813	-10.994	-0.180
FeCl2+	1.195e-011	1.076e-011	-10.923	-10.968	-0.045
Fe(OH)4-	7.456e-012	6.715e-012	-11.127	-11.173	-0.045
FeCl4-	2.465e-020	2.220e-020	-19.608	-19.654	-0.045
H(0)	2.087e-036				
H2	1.043e-036	1.046e-036	-35.982	-35.980	0.001
K	6.487e-004				
K+	6.402e-004	5.747e-004	-3.194	-3.241	-0.047
KSO4-	8.462e-006	7.621e-006	-5.073	-5.118	-0.045
KCl	2.528e-008	2.528e-008	-7.597	-7.597	0.000
KHSO4	2.441e-010	2.441e-010	-9.612	-9.612	0.000
KOH	5.487e-014	5.487e-014	-13.261	-13.261	0.000
Mg	1.519e-004				
Mg+2	1.167e-004	8.003e-005	-3.933	-4.097	-0.164
MgSO4	3.511e-005	3.511e-005	-4.455	-4.455	0.000
MgCl+	9.088e-008	8.185e-008	-7.042	-7.087	-0.045
Mg4(OH)4+4	2.116e-038	4.195e-039	-37.675	-38.377	-0.703
Mn(2)	9.269e-005				
Mn+2	7.252e-005	4.870e-005	-4.140	-4.312	-0.173
MnSO4	1.974e-005	1.974e-005	-4.705	-4.705	0.000
MnNO3+	2.744e-007	2.471e-007	-6.562	-6.607	-0.045
MnCl+	1.508e-007	1.358e-007	-6.821	-6.867	-0.045
Mn(NO3)2	1.987e-009	1.987e-009	-8.702	-8.702	0.000
MnOH+	3.828e-011	3.447e-011	-10.417	-10.463	-0.045
MnCl3-	5.654e-014	5.092e-014	-13.248	-13.293	-0.045
Mn2OH+3	4.527e-015	1.799e-015	-14.344	-14.745	-0.401
Mn(OH)2	2.330e-018	2.330e-018	-17.633	-17.633	0.000
Mn2(OH)3+	6.924e-020	6.236e-020	-19.160	-19.205	-0.045
Mn(OH)3-	6.684e-026	6.019e-026	-25.175	-25.220	-0.045
Mn(OH)4-2	2.140e-035	1.404e-035	-34.670	-34.853	-0.183
Mn(3)	3.269e-018				
Mn+3	3.269e-018	1.299e-018	-17.486	-17.886	-0.401
Mn(6)	8.780e-040				
MnO4-2	8.780e-040	5.759e-040	-39.057	-39.240	-0.183
Mn(7)	2.820e-037				
MnO4-	2.820e-037	2.536e-037	-36.550	-36.596	-0.046
N(5)	3.576e-003				
NO3-	3.566e-003	3.202e-003	-2.448	-2.495	-0.047
CaNO3+	9.050e-006	8.150e-006	-5.043	-5.089	-0.045
MnNO3+	2.744e-007	2.471e-007	-6.562	-6.607	-0.045

HNO3	6.080e-009	6.080e-009	-8.216	-8.216	0.000
FeNO3+2	2.255e-009	1.488e-009	-8.647	-8.827	-0.180
Mn(NO3)2	1.987e-009	1.987e-009	-8.702	-8.702	0.000
Na	7.877e-004				
Na+	7.790e-004	7.016e-004	-3.108	-3.154	-0.045
NaSO4-	8.456e-006	7.615e-006	-5.073	-5.118	-0.045
NaCl	1.615e-007	1.615e-007	-6.792	-6.792	0.000
NaOH	3.212e-014	3.212e-014	-13.493	-13.493	0.000
NaAlO2	8.641e-015	8.641e-015	-14.063	-14.063	0.000
O(0)	1.161e-020				
O2	5.803e-021	5.818e-021	-20.236	-20.235	0.001
S(6)	2.727e-003				
SO4-2	2.505e-003	1.643e-003	-2.601	-2.784	-0.183
CaSO4	1.219e-004	1.219e-004	-3.914	-3.914	0.000
MgSO4	3.511e-005	3.511e-005	-4.455	-4.455	0.000
MnSO4	1.974e-005	1.974e-005	-4.705	-4.705	0.000
AlSO4+	1.615e-005	1.455e-005	-4.792	-4.837	-0.045
KSO4-	8.462e-006	7.621e-006	-5.073	-5.118	-0.045
NaSO4-	8.456e-006	7.615e-006	-5.073	-5.118	-0.045
HSO4-	6.690e-006	6.025e-006	-5.175	-5.220	-0.045
Al(SO4)2-	2.060e-006	1.855e-006	-5.686	-5.732	-0.045
ZnSO4	1.610e-006	1.610e-006	-5.793	-5.793	0.000
CuSO4	4.117e-007	4.117e-007	-6.385	-6.385	0.000
FeSO4	1.262e-007	1.262e-007	-6.899	-6.899	0.000
FeSO4+	8.205e-009	7.389e-009	-8.086	-8.131	-0.045
KHSO4	2.441e-010	2.441e-010	-9.612	-9.612	0.000
Fe(SO4)2-	2.279e-010	2.052e-010	-9.642	-9.688	-0.045
H2SO4	2.064e-013	2.064e-013	-12.685	-12.685	0.000
Zn	8.568e-006				
Zn+2	6.946e-006	4.665e-006	-5.158	-5.331	-0.173
ZnSO4	1.610e-006	1.610e-006	-5.793	-5.793	0.000
ZnCl+	1.140e-008	1.027e-008	-7.943	-7.989	-0.045
ZnOH+	1.564e-010	1.409e-010	-9.806	-9.851	-0.045
ZnCl2	1.571e-011	1.571e-011	-10.804	-10.804	0.000
Zn(OH)Cl	4.834e-012	4.834e-012	-11.316	-11.316	0.000
Zn(OH)2	1.661e-014	1.661e-014	-13.780	-13.780	0.000
ZnCl3-	1.262e-014	1.136e-014	-13.899	-13.944	-0.045
ZnCl4-2	1.720e-016	1.128e-016	-15.764	-15.948	-0.183
Zn(OH)3-	1.575e-021	1.418e-021	-20.803	-20.848	-0.045
Zn(OH)4-2	1.015e-029	6.658e-030	-28.994	-29.177	-0.183
ZnClO4+	0.000e+000	0.000e+000	-63.087	-63.133	-0.045

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

Phase	SI	log IAP	log KT	
Al	-126.48	23.43	149.91	Al
Al(g)	-177.18	23.43	200.62	Al
Al2(SO4)3	-37.38	-18.48	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-20.04	-18.48	1.56	Al2(SO4)3:6H2O
Alum-K	-8.90	-13.87	-4.97	KAl(SO4)2:12H2O
Alunite	3.11	2.64	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.73	-6.08	-4.35	CaSO4
Antarcticite	-13.15	-9.06	4.09	CaCl2:6H2O
Antlerite	-11.64	-2.91	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.56	-18.44	-3.89	NaK3(SO4)2
Arcanite	-7.42	-9.27	-1.84	K2SO4
Arsenolite	-43.72	-63.56	-19.84	As2O3
As	-59.29	-16.60	42.68	As
As2O5	-24.87	-22.73	2.14	As2O5
As4O6(cubi)	-87.29	-127.12	-39.82	As4O6
As4O6(mono)	-87.07	-127.12	-40.05	As4O6
Atacamite	-17.23	-2.97	14.26	Cu4Cl2(OH)6
Bassanite	-2.37	-6.08	-3.71	CaSO4:0.5H2O
Birnessite	-35.98	-121.52	-85.55	Mn8O14:5H2O
Bischofite	-14.25	-9.86	4.39	MgCl2:6H2O
Bixbyite	-8.17	-9.13	-0.96	Mn2O3

Bloedite	-13.50	-15.97	-2.48	Na2Mg(SO4)2·4H2O
Boehmite	0.71	8.26	7.55	AlO2H
Brochantite	-15.41	0.01	15.42	Cu4(SO4)(OH)6
Brucite	-11.50	4.78	16.28	Mg(OH)2
Ca	-124.13	15.70	139.83	Ca
Ca(g)	-149.37	15.70	165.07	Ca
Ca2Al2O5·8H2O	-31.88	27.69	59.57	Ca2Al2O5·8H2O
Ca2Cl2(OH)2·H2O	-29.76	-3.47	26.29	Ca2Cl2(OH)2·H2O
Ca3(AsO4)2	-23.78	-5.97	17.80	Ca3(AsO4)2
Ca3Al2O6	-79.76	33.27	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-89.65	50.83	140.48	Ca4Al2Fe2O10
Ca4Al2O7·13H2O	-68.40	38.86	107.25	Ca4Al2O7·13H2O
Ca4Al2O7·19H2O	-64.83	38.86	103.68	Ca4Al2O7·19H2O
Ca4Cl2(OH)6·13H2O	-60.63	7.70	68.33	Ca4Cl2(OH)6·13H2O
CaAl2O4	-24.81	22.10	46.91	CaAl2O4
CaAl2O4·10H2O	-15.90	22.10	37.99	CaAl2O4·10H2O
CaAl4O7	-29.98	38.61	68.59	CaAl4O7
Carnallite	-20.26	-15.99	4.27	KMgCl3·6H2O
CaSO4·0.5H2O(beta)	-2.54	-6.08	-3.54	CaSO4·0.5H2O
Chalcanthite	-6.12	-8.75	-2.63	CuSO4·5H2O
Chalcocyanite	-11.66	-8.75	2.91	CuSO4
Chloromagnesite	-31.68	-9.86	21.82	MgCl2
Cl2(g)	-27.76	-24.76	2.99	Cl2
Claudetite	-43.76	-63.56	-19.80	As2O3
Corundum	-1.78	16.51	18.29	Al2O3
Cu	-18.46	13.04	31.50	Cu
Cu(g)	-70.62	13.04	83.66	Cu
CuCl2	-15.45	-11.73	3.72	CuCl2
Cuprite	-19.66	-21.57	-1.91	Cu2O
Delafossite	1.64	-4.80	-6.44	CuFeO2
Diaspore	1.11	8.26	7.15	AlHO2
Epsomite	-4.92	-6.88	-1.96	MgSO4·7H2O
Ettringite	-47.43	15.03	62.46	Ca6Al2(SO4)3(OH)12·26H2O
Fe	-46.33	12.68	59.02	Fe
Fe(OH)2	-11.33	2.57	13.89	Fe(OH)2
Fe(OH)3	0.35	5.99	5.64	Fe(OH)3
Fe2(SO4)3	-26.07	-23.02	3.05	Fe2(SO4)3
FeO	-10.96	2.57	13.52	FeO
Ferrite-Ca	-3.94	17.56	21.50	CaFe2O4
Ferrite-Cu	4.61	14.89	10.28	CuFe2O4
Ferrite-Dicalcium	-33.65	23.15	56.80	Ca2Fe2O5
Ferrite-Mg	-4.26	16.76	21.02	MgFe2O4
Ferrite-Zn	3.82	15.52	11.70	ZnFe2O4
FeSO4	-11.71	-9.10	2.61	FeSO4
Gibbsite	0.52	8.26	7.74	Al(OH)3
Glauberite	-9.70	-15.17	-5.47	Na2Ca(SO4)2
Goethite	5.46	5.99	0.53	FeOOH
Gypsum	-1.55	-6.08	-4.53	CaSO4·2H2O
H2(g)	-32.88	-35.98	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.60	-6.04	1.56	NaCl
Hausmannite	-14.71	-4.57	10.14	Mn3O4
HCl(g)	-13.62	-7.32	6.30	HCl
Hematite	11.90	11.97	0.08	Fe2O3
Hercynite	-9.72	19.08	28.80	FeAl2O4
Hexahydrite	-5.15	-6.88	-1.73	MgSO4·6H2O
Hydrophilite	-20.81	-9.06	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	5.24	-4.17	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	1.37	-4.08	-5.45	NaFe3(SO4)2(OH)6
K	-64.72	6.26	70.98	K
K(g)	-75.32	6.26	81.58	K
K2O	-81.64	2.40	84.04	K2O
K3H(SO4)2	-16.11	-19.73	-3.62	K3H(SO4)2
Kainite	-12.69	-13.00	-0.31	KMgClSO4·3H2O
KAl(SO4)2	-17.14	-13.87	3.27	KAl(SO4)2
Katoite	-45.67	33.27	78.94	Ca3Al2H12O12

Kieserite	-6.61	-6.88	-0.27	MgSO4:H2O
KMgCl3	-37.23	-15.99	21.25	KMgCl3
KMgCl3:2H2O	-29.95	-15.99	13.96	KMgCl3:2H2O
Lammerite	-15.53	-13.97	1.55	Cu3(AsO4)2
Lawrencite	-21.13	-12.08	9.05	FeCl2
Leonite	-12.03	-16.15	-4.11	K2Mg(SO4)2:4H2O
Lime	-26.98	5.59	32.57	CaO
Magnetite	4.12	14.54	10.42	Fe3O4
Manganite	-4.40	-4.57	-0.16	MnO(OH)
Manganosite	-13.35	4.57	17.92	MnO
Mayenite	-311.52	182.63	494.15	Ca12Al14O33
Melanterite	-6.70	-9.10	-2.40	FeSO4:7H2O
Mercallite	-9.03	-10.46	-1.44	KHSO4
Mg	-107.62	14.90	122.52	Mg
Mg(g)	-127.34	14.90	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.88	-5.69	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-13.70	-4.49	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.59	-9.86	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.16	-9.86	7.30	MgCl2:4H2O
MgCl2:H2O	-25.93	-9.86	16.07	MgCl2:H2O
MgOHCl	-18.43	-2.54	15.89	MgOHCl
MgSO4	-11.71	-6.88	4.83	MgSO4
Mirabilite	-7.94	-9.09	-1.15	Na2SO4:10H2O
Misenite	-60.98	-72.06	-11.08	K8H6(SO4)7
Mn	-68.25	14.69	82.93	Mn
Mn(OH)2(am)	-10.74	4.57	15.31	Mn(OH)2
Mn(OH)3	-10.91	-4.57	6.34	Mn(OH)3
MnCl2:2H2O	-14.08	-10.08	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.83	-10.08	2.75	MnCl2:4H2O
MnCl2:H2O	-15.62	-10.08	5.54	MnCl2:H2O
MnO2(gamma)	-5.65	-21.78	-16.13	MnO2
MnSO4	-9.71	-7.10	2.61	MnSO4
Molysite	-29.45	-15.98	13.47	FeCl3
Na	-61.03	6.34	67.37	Na
Na(g)	-74.51	6.34	80.86	Na
Na2O	-64.85	2.57	67.42	Na2O
Na3H(SO4)2	-18.58	-19.47	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-18.37	-24.26	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-12.61	7.27	19.88	NaFeO2
Nantokite	-11.34	-18.11	-6.77	CuCl
Niter	-5.51	-5.74	-0.22	KNO3
NO2(g)	-10.22	-1.88	8.35	NO2
O2(g)	-17.34	-20.24	-2.89	O2
Oxychloride-Mg	-23.59	2.24	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-5.49	-6.88	-1.39	MgSO4:5H2O
Periclase	-16.54	4.78	21.33	MgO
Picromerite	-11.71	-16.15	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-13.99	-28.30	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-16.96	5.59	22.55	Ca(OH)2
Pyrolusite	-4.12	-21.78	-17.66	MnO2
Scacchite	-18.82	-10.08	8.74	MnCl2
Spinel	-16.31	21.30	37.61	Al2MgO4
Starkeyite	-5.88	-6.88	-1.00	MgSO4:4H2O
Sylvite	-6.95	-6.12	0.83	KCl
Syngenite	-7.74	-15.34	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.93	-28.79	17.14	Mg2CaCl6:12H2O
Tenorite	-4.73	2.92	7.65	CuO
Thenardite	-8.73	-9.09	-0.36	Na2SO4
Todorokite	-29.69	-75.52	-45.82	Mn7O12:3H2O
Wustite	-9.61	2.79	12.40	Fe.947O
Zincite	-7.65	3.55	11.20	ZnO
Zn	-55.12	13.67	68.79	Zn
Zn(ClO4)2:6H2O	-129.12	-123.49	5.63	Zn(ClO4)2:6H2O
Zn(g)	-71.74	13.67	85.41	Zn
Zn(NO3)2:6H2O	-13.72	-10.32	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-8.38	3.55	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-8.11	3.55	11.66	Zn(OH)2

Zn(OH)2(gamma)	-8.33	3.55	11.88	Zn(OH)2
Zn2(OH)3Cl	-15.52	-0.23	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-12.15	-4.57	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-21.40	-12.08	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-31.77	-12.68	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-38.79	3.87	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.18	-11.10	7.08	ZnCl2
ZnSO4	-11.65	-8.12	3.53	ZnSO4
ZnSO4:6H2O	-6.42	-8.12	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-6.24	-8.12	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-7.56	-8.12	-0.55	ZnSO4:H2O

Initial solution 2. UGA2

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

Elements	Molality	Moles
Al	7.166e-004	7.166e-004
As	9.097e-006	9.097e-006
C(4)	2.004e-005	2.004e-005
Ca	8.488e-004	8.488e-004
Cl	1.005e-003	1.005e-003
Cu	3.785e-007	3.785e-007
Fe	1.795e-003	1.795e-003
K	3.691e-005	3.691e-005
Mg	9.567e-004	9.567e-004
Mn	1.345e-004	1.345e-004
N(5)	3.481e-003	3.481e-003
Na	3.601e-004	3.601e-004
S(6)	2.058e-002	2.058e-002
Zn	4.292e-005	4.292e-005

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

pH	=	2.460
pe	=	12.000
Activity of water	=	0.999
Ionic strength	=	4.285e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	-7.643e-003
Total CO2 (mol/kg)	=	2.004e-005
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-2.830e-002
Percent error, 100*(Cat- An)/(Cat+ An)	=	-58.21
Iterations	=	8
Total H	=	1.110579e+002
Total O	=	5.561835e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.017e-003	3.467e-003	-2.396	-2.460	-0.064
OH-	3.368e-012	2.777e-012	-11.473	-11.556	-0.084
H2O	5.553e+001	9.995e-001	1.744	-0.000	0.000
Al	7.166e-004				
AlSO4+	3.590e-004	2.976e-004	-3.445	-3.526	-0.081
Al(SO4)2-	1.998e-004	1.656e-004	-3.699	-3.781	-0.081
Al+3	1.575e-004	4.057e-005	-3.803	-4.392	-0.589
AlOH+2	2.753e-007	1.310e-007	-6.560	-6.883	-0.322
Al(OH)2+	1.058e-010	8.769e-011	-9.976	-10.057	-0.081
Al2(OH)2+4	4.747e-011	2.791e-012	-10.324	-11.554	-1.231
HALO2	3.681e-014	3.681e-014	-13.434	-13.434	0.000
Al3(OH)4+5	4.580e-016	6.074e-018	-15.339	-17.217	-1.877
ALO2-	4.386e-018	3.636e-018	-17.358	-17.439	-0.081

NaAlO2	1.977e-022	1.977e-022	-21.704	-21.704	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-73.428	-77.110	-3.681
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-106.650	-106.650	0.000
As(3)	2.138e-015				
HAsO2	1.141e-015	1.141e-015	-14.943	-14.943	0.000
As(OH)3	9.969e-016	9.969e-016	-15.001	-15.001	0.000
H2AsO3-	2.121e-022	1.758e-022	-21.673	-21.755	-0.081
AsO2-	2.029e-022	1.682e-022	-21.693	-21.774	-0.081
AsO2OH-2	1.062e-030	4.955e-031	-29.974	-30.305	-0.331
As(5)	9.097e-006				
H2AsO4-	6.039e-006	5.006e-006	-5.219	-5.301	-0.081
H3AsO4	3.057e-006	3.057e-006	-5.515	-5.515	0.000
HAsO4-2	5.137e-010	2.397e-010	-9.289	-9.620	-0.331
AsO4-3	9.905e-019	1.773e-019	-18.004	-18.751	-0.747
C(4)	2.004e-005				
CO2	2.004e-005	2.025e-005	-4.698	-4.694	0.005
HCO3-	3.036e-009	2.516e-009	-8.518	-8.599	-0.081
FeHCO3+	7.141e-010	5.920e-010	-9.146	-9.228	-0.081
CaHCO3+	9.995e-012	8.286e-012	-11.000	-11.082	-0.081
FeCO3+	9.641e-012	7.992e-012	-11.016	-11.097	-0.081
MgHCO3+	8.905e-012	7.383e-012	-11.050	-11.132	-0.081
NaHCO3	1.026e-012	1.026e-012	-11.989	-11.989	0.000
ZnHCO3+	9.600e-013	7.958e-013	-12.018	-12.099	-0.081
MnHCO3+	8.251e-013	6.840e-013	-12.084	-12.165	-0.081
FeCO3	8.194e-016	8.194e-016	-15.086	-15.086	0.000
CO3-2	6.764e-017	3.220e-017	-16.170	-16.492	-0.322
MnCO3	4.024e-017	4.024e-017	-16.395	-16.395	0.000
CuCO3	3.198e-017	3.198e-017	-16.495	-16.495	0.000
CaCO3	2.073e-017	2.073e-017	-16.683	-16.683	0.000
MgCO3	8.603e-018	8.603e-018	-17.065	-17.065	0.000
ZnCO3	3.317e-018	3.317e-018	-17.479	-17.479	0.000
NaCO3-	3.873e-020	3.211e-020	-19.412	-19.493	-0.081
Cu(CO3)2-2	3.931e-030	1.834e-030	-29.405	-29.737	-0.331
CuCO3(OH)2-2	4.841e-032	2.259e-032	-31.315	-31.646	-0.331
Ca	8.488e-004				
Ca+2	5.530e-004	2.778e-004	-3.257	-3.556	-0.299
CaSO4	2.909e-004	2.909e-004	-3.536	-3.536	0.000
CaNO3+	4.784e-006	3.966e-006	-5.320	-5.402	-0.081
CaCl+	5.848e-008	4.848e-008	-7.233	-7.314	-0.081
CaCl2	4.695e-011	4.695e-011	-10.328	-10.328	0.000
CaHCO3+	9.995e-012	8.286e-012	-11.000	-11.082	-0.081
CaOH+	1.365e-014	1.131e-014	-13.865	-13.946	-0.081
CaCO3	2.073e-017	2.073e-017	-16.683	-16.683	0.000
Cl(-1)	1.005e-003				
Cl-	1.004e-003	8.233e-004	-2.998	-3.084	-0.086
HCl	6.411e-007	6.411e-007	-6.193	-6.193	0.000
FeCl+	3.243e-007	2.689e-007	-6.489	-6.570	-0.081
MgCl+	1.958e-007	1.623e-007	-6.708	-6.790	-0.081
MnCl+	7.549e-008	6.258e-008	-7.122	-7.204	-0.081
CaCl+	5.848e-008	4.848e-008	-7.233	-7.314	-0.081
NaCl	4.124e-008	4.124e-008	-7.385	-7.385	0.000
ZnCl+	2.047e-008	1.697e-008	-7.689	-7.770	-0.081
FeCl+2	1.239e-008	5.896e-009	-7.907	-8.229	-0.322
FeCl2+	4.740e-009	3.930e-009	-8.324	-8.406	-0.081
KCl	7.915e-010	7.915e-010	-9.102	-9.102	0.000
CuCl+	2.829e-010	2.345e-010	-9.548	-9.630	-0.081
CaCl2	4.695e-011	4.695e-011	-10.328	-10.328	0.000
ZnCl2	1.632e-011	1.632e-011	-10.787	-10.787	0.000
FeCl2	1.188e-012	1.188e-012	-11.925	-11.925	0.000
CuCl2	1.017e-013	1.017e-013	-12.993	-12.993	0.000
Zn(OH)Cl	8.364e-014	8.364e-014	-13.078	-13.078	0.000
MnCl3-	1.118e-014	9.266e-015	-13.952	-14.033	-0.081
ZnCl3-	8.950e-015	7.420e-015	-14.048	-14.130	-0.081
ZnCl4-2	9.924e-017	4.630e-017	-16.003	-16.334	-0.331
FeCl4-2	4.986e-018	2.326e-018	-17.302	-17.633	-0.331
FeCl4-	3.863e-018	3.202e-018	-17.413	-17.495	-0.081

CuCl2-	3.088e-018	2.560e-018	-17.510	-17.592	-0.081
CuCl3-2	2.901e-020	1.353e-020	-19.537	-19.869	-0.331
CuCl4-2	2.772e-024	1.293e-024	-23.557	-23.888	-0.331
Cl(1)	6.855e-028				
HClO	6.855e-028	6.855e-028	-27.164	-27.164	0.000
ClO-	6.431e-033	5.331e-033	-32.192	-32.273	-0.081
Cl(3)	0.000e+000				
HClO2	0.000e+000	0.000e+000	-53.647	-53.647	0.000
ClO2-	0.000e+000	0.000e+000	-54.275	-54.357	-0.081
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-62.504	-62.588	-0.084
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-75.037	-75.120	-0.084
ZnClO4+	0.000e+000	0.000e+000	-78.673	-78.755	-0.081
Cu(1)	7.188e-017				
Cu+	6.876e-017	5.700e-017	-16.163	-16.244	-0.081
CuCl2-	3.088e-018	2.560e-018	-17.510	-17.592	-0.081
CuCl3-2	2.901e-020	1.353e-020	-19.537	-19.869	-0.331
Cu(2)	3.785e-007				
Cu+2	2.072e-007	1.041e-007	-6.684	-6.982	-0.299
CuSO4	1.710e-007	1.710e-007	-6.767	-6.767	0.000
CuCl+	2.829e-010	2.345e-010	-9.548	-9.630	-0.081
CuOH+	1.868e-012	1.548e-012	-11.729	-11.810	-0.081
CuCl2	1.017e-013	1.017e-013	-12.993	-12.993	0.000
CuCO3	3.198e-017	3.198e-017	-16.495	-16.495	0.000
CuCl4-2	2.772e-024	1.293e-024	-23.557	-23.888	-0.331
Cu(CO3)2-2	3.931e-030	1.834e-030	-29.405	-29.737	-0.331
CuCO3(OH)2-2	4.841e-032	2.259e-032	-31.315	-31.646	-0.331
CuO2-2	5.476e-037	2.555e-037	-36.262	-36.593	-0.331
Fe(2)	1.402e-003				
Fe+2	8.921e-004	4.483e-004	-3.050	-3.348	-0.299
FeSO4	5.093e-004	5.093e-004	-3.293	-3.293	0.000
FeCl+	3.243e-007	2.689e-007	-6.489	-6.570	-0.081
FeHCO3+	7.141e-010	5.920e-010	-9.146	-9.228	-0.081
FeOH+	4.929e-011	4.086e-011	-10.307	-10.389	-0.081
FeCl2	1.188e-012	1.188e-012	-11.925	-11.925	0.000
FeCO3	8.194e-016	8.194e-016	-15.086	-15.086	0.000
FeCl4-2	4.986e-018	2.326e-018	-17.302	-17.633	-0.331
Fe(OH)2	9.355e-020	9.355e-020	-19.029	-19.029	0.000
Fe(OH)3-	1.295e-027	1.074e-027	-26.888	-26.969	-0.081
Fe(OH)4-2	6.632e-040	3.094e-040	-39.178	-39.509	-0.331
Fe(3)	3.929e-004				
FeOH+2	1.680e-004	7.999e-005	-3.775	-4.097	-0.322
Fe+3	1.668e-004	4.298e-005	-3.778	-4.367	-0.589
FeSO4+	3.596e-005	2.981e-005	-4.444	-4.526	-0.081
Fe(OH)2+	9.209e-006	7.635e-006	-5.036	-5.117	-0.081
Fe(SO4)2-	4.358e-006	3.612e-006	-5.361	-5.442	-0.081
Fe2(OH)2+4	2.929e-006	1.722e-007	-5.533	-6.764	-1.231
FeNO3+2	2.572e-006	1.224e-006	-5.590	-5.912	-0.322
Fe3(OH)4+5	2.071e-008	2.747e-010	-7.684	-9.561	-1.877
FeCl+2	1.239e-008	5.896e-009	-7.907	-8.229	-0.322
FeCl2+	4.740e-009	3.930e-009	-8.324	-8.406	-0.081
Fe(OH)3	1.029e-009	1.029e-009	-8.987	-8.987	0.000
FeCO3+	9.641e-012	7.992e-012	-11.016	-11.097	-0.081
Fe(OH)4-	8.990e-017	7.453e-017	-16.046	-16.128	-0.081
FeCl4-	3.863e-018	3.202e-018	-17.413	-17.495	-0.081
H(0)	1.888e-032				
H2	9.442e-033	9.540e-033	-32.025	-32.020	0.005
K	3.691e-005				
K+	3.491e-005	2.863e-005	-4.457	-4.543	-0.086
KSO4-	1.998e-006	1.656e-006	-5.699	-5.781	-0.081
KHSO4	5.067e-009	5.067e-009	-8.295	-8.295	0.000
KCl	7.915e-010	7.915e-010	-9.102	-9.102	0.000
KOH	2.861e-017	2.861e-017	-16.543	-16.543	0.000
Mg	9.567e-004				
MgSO4	4.835e-004	4.835e-004	-3.316	-3.316	0.000
Mg+2	4.730e-004	2.526e-004	-3.325	-3.598	-0.272

MgCl+	1.958e-007	1.623e-007	-6.708	-6.790	-0.081
MgHCO3+	8.905e-012	7.383e-012	-11.050	-11.132	-0.081
MgCO3	8.603e-018	8.603e-018	-17.065	-17.065	0.000
Mg4(OH)4+4	0.000e+000	0.000e+000	-43.071	-44.301	-1.231
Mn(2)	1.345e-004				
Mn+2	7.105e-005	3.570e-005	-4.148	-4.447	-0.299
MnSO4	6.314e-005	6.314e-005	-4.200	-4.200	0.000
MnNO3+	1.944e-007	1.611e-007	-6.711	-6.793	-0.081
MnCl+	7.549e-008	6.258e-008	-7.122	-7.204	-0.081
Mn(NO3)2	1.153e-009	1.153e-009	-8.938	-8.938	0.000
MnHCO3+	8.251e-013	6.840e-013	-12.084	-12.165	-0.081
MnOH+	3.190e-013	2.645e-013	-12.496	-12.578	-0.081
MnCl3-	1.118e-014	9.266e-015	-13.952	-14.033	-0.081
Mn2OH+3	5.178e-017	1.012e-017	-16.286	-16.995	-0.709
MnCO3	4.024e-017	4.024e-017	-16.395	-16.395	0.000
Mn(OH)2	1.871e-022	1.871e-022	-21.728	-21.728	0.000
Mn2(OH)3+	4.635e-026	3.842e-026	-25.334	-25.415	-0.081
Mn(OH)3-	6.104e-032	5.060e-032	-31.214	-31.296	-0.081
Mn(OH)4-2	0.000e+000	0.000e+000	-42.577	-42.908	-0.331
Mn(3)	4.873e-018				
Mn+3	4.873e-018	9.522e-019	-17.312	-18.021	-0.709
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-54.884	-55.215	-0.331
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-52.488	-52.571	-0.084
N(5)	3.481e-003				
NO3-	3.473e-003	2.848e-003	-2.459	-2.545	-0.086
CaNO3+	4.784e-006	3.966e-006	-5.320	-5.402	-0.081
FeNO3+2	2.572e-006	1.224e-006	-5.590	-5.912	-0.322
HNO3	5.165e-007	5.165e-007	-6.287	-6.287	0.000
MnNO3+	1.944e-007	1.611e-007	-6.711	-6.793	-0.081
Mn(NO3)2	1.153e-009	1.153e-009	-8.938	-8.938	0.000
Na	3.601e-004				
Na+	3.438e-004	2.850e-004	-3.464	-3.545	-0.081
NaSO4-	1.628e-005	1.350e-005	-4.788	-4.870	-0.081
NaCl	4.124e-008	4.124e-008	-7.385	-7.385	0.000
NaHCO3	1.026e-012	1.026e-012	-11.989	-11.989	0.000
NaOH	1.365e-016	1.365e-016	-15.865	-15.865	0.000
NaCO3-	3.873e-020	3.211e-020	-19.412	-19.493	-0.081
NaAlO2	1.977e-022	1.977e-022	-21.704	-21.704	0.000
O(0)	1.384e-028				
O2	6.918e-029	6.990e-029	-28.160	-28.156	0.005
S(6)	2.058e-002				
SO4-2	1.536e-002	7.168e-003	-1.814	-2.145	-0.331
HSO4-	3.029e-003	2.511e-003	-2.519	-2.600	-0.081
FeSO4	5.093e-004	5.093e-004	-3.293	-3.293	0.000
MgSO4	4.835e-004	4.835e-004	-3.316	-3.316	0.000
AlSO4+	3.590e-004	2.976e-004	-3.445	-3.526	-0.081
CaSO4	2.909e-004	2.909e-004	-3.536	-3.536	0.000
Al(SO4)2-	1.998e-004	1.656e-004	-3.699	-3.781	-0.081
MnSO4	6.314e-005	6.314e-005	-4.200	-4.200	0.000
FeSO4+	3.596e-005	2.981e-005	-4.444	-4.526	-0.081
ZnSO4	1.848e-005	1.848e-005	-4.733	-4.733	0.000
NaSO4-	1.628e-005	1.350e-005	-4.788	-4.870	-0.081
Fe(SO4)2-	4.358e-006	3.612e-006	-5.361	-5.442	-0.081
KSO4-	1.998e-006	1.656e-006	-5.699	-5.781	-0.081
CuSO4	1.710e-007	1.710e-007	-6.767	-6.767	0.000
H2SO4	8.213e-009	8.213e-009	-8.085	-8.085	0.000
KHSO4	5.067e-009	5.067e-009	-8.295	-8.295	0.000
Zn	4.292e-005				
Zn+2	2.442e-005	1.227e-005	-4.612	-4.911	-0.299
ZnSO4	1.848e-005	1.848e-005	-4.733	-4.733	0.000
ZnCl+	2.047e-008	1.697e-008	-7.689	-7.770	-0.081
ZnCl2	1.632e-011	1.632e-011	-10.787	-10.787	0.000
ZnOH+	4.678e-012	3.878e-012	-11.330	-11.411	-0.081
ZnHCO3+	9.600e-013	7.958e-013	-12.018	-12.099	-0.081
Zn(OH)Cl	8.364e-014	8.364e-014	-13.078	-13.078	0.000

ZnCl3-	8.950e-015	7.420e-015	-14.048	-14.130	-0.081
ZnCl4-2	9.924e-017	4.630e-017	-16.003	-16.334	-0.331
Zn(OH)2	4.788e-018	4.788e-018	-17.320	-17.320	0.000
ZnCO3	3.317e-018	3.317e-018	-17.479	-17.479	0.000
Zn(OH)3-	5.160e-027	4.277e-027	-26.287	-26.369	-0.081
Zn(OH)4-2	4.505e-037	2.102e-037	-36.346	-36.677	-0.331
ZnClO4+	0.000e+000	0.000e+000	-78.673	-78.755	-0.081

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

Phase	SI	log IAP	log KT	
Al	-125.81	24.10	149.91	Al
Al(g)	-176.51	24.10	200.62	Al
Al2(SO4)3	-34.12	-15.22	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.77	-15.22	1.56	Al2(SO4)3:6H2O
Alum-K	-8.26	-13.23	-4.97	KAl(SO4)2:12H2O
Alunite	-6.78	-7.25	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.35	-5.70	-4.35	CaSO4
Antarcticite	-13.82	-9.73	4.09	CaCl2:6H2O
Antlerite	-21.98	-13.25	8.73	Cu3(SO4)(OH)4
Aphthitalite	-17.58	-21.46	-3.89	NaK3(SO4)2
Aragonite	-11.67	-9.70	1.97	CaCO3
Arcanite	-9.39	-11.23	-1.84	K2SO4
Arsenolite	-28.59	-48.43	-19.84	As2O3
Artinite	-28.04	-8.42	19.63	Mg2CO3(OH)2:3H2O
As	-45.78	-3.10	42.68	As
As2O5	-17.66	-15.52	2.14	As2O5
As4O6(cubi)	-57.03	-96.86	-39.82	As4O6
As4O6(mono)	-56.81	-96.86	-40.05	As4O6
Atacamite	-33.60	-19.34	14.26	Cu4Cl2(OH)6
Azurite	-37.42	-28.31	9.12	Cu3(CO3)2(OH)2
Bassanite	-1.99	-5.70	-3.71	CaSO4:0.5H2O
Birnessite	-92.50	-178.04	-85.55	Mn8O14:5H2O
Bischofite	-14.16	-9.77	4.39	MgCl2:6H2O
Bixbyite	-20.32	-21.28	-0.96	Mn2O3
Bloedite	-12.50	-14.98	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-4.56	2.99	7.55	AlO2H
Brochantite	-30.74	-15.32	15.42	Cu4(SO4)(OH)6
Brucite	-14.96	1.32	16.28	Mg(OH)2
Burkeite	-41.19	-31.70	9.49	Na6CO3(SO4)2
C	-47.05	17.10	64.15	C
C(g)	-164.67	17.10	181.77	C
Ca	-124.39	15.44	139.83	Ca
Ca(g)	-149.63	15.44	165.07	Ca
Ca2Al2O5:8H2O	-50.87	8.70	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-34.65	-8.36	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-29.23	-11.43	17.80	Ca3(AsO4)2
Ca3Al2O6	-102.97	10.07	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-123.03	17.46	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-95.83	11.43	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-92.26	11.43	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-73.97	-5.64	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-39.57	7.34	46.91	CaAl2O4
CaAl2O4:10H2O	-30.66	7.34	37.99	CaAl2O4:10H2O
CaAl4O7	-55.28	13.32	68.59	CaAl4O7
Calcite	-11.52	-9.70	1.82	CaCO3
Carnallite	-21.67	-17.40	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.17	-5.70	-3.54	CaSO4:0.5H2O
Chalcanthite	-6.50	-9.13	-2.63	CuSO4:5H2O
Chalcocyanite	-12.04	-9.13	2.91	CuSO4
Chloromagnesite	-31.58	-9.77	21.82	MgCl2
Cl2(g)	-28.16	-25.17	2.99	Cl2
Claudetite	-28.63	-48.43	-19.80	As2O3
CO2(g)	-3.23	-11.06	-7.83	CO2
Corundum	-12.32	5.98	18.29	Al2O3
Cu	-19.48	12.02	31.50	Cu

Cu(g)	-71.64	12.02	83.66	Cu
CuCl2	-16.87	-13.15	3.72	CuCl2
Cuprite	-25.66	-27.57	-1.91	Cu2O
Dawsonite	-13.50	-9.16	4.34	NaAlCO3(OH)2
Delafossite	-4.34	-10.77	-6.44	CuFeO2
Diaspore	-4.16	2.99	7.15	AlHO2
Dolomite	-21.91	-19.43	2.47	CaMg(CO3)2
Dolomite-dis	-23.44	-19.43	4.01	CaMg(CO3)2
Dolomite-ord	-21.90	-19.43	2.46	CaMg(CO3)2
Epsomite	-3.78	-5.74	-1.96	MgSO4:7H2O
Ettringite	-69.51	-7.04	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-43.37	15.65	59.02	Fe
Fe(OH)2	-12.32	1.57	13.89	Fe(OH)2
Fe(OH)3	-2.63	3.01	5.64	Fe(OH)3
Fe2(SO4)3	-18.21	-15.17	3.05	Fe2(SO4)3
FeO	-11.95	1.57	13.52	FeO
Ferrite-Ca	-14.11	7.39	21.50	CaFe2O4
Ferrite-Cu	-6.32	3.96	10.28	CuFe2O4
Ferrite-Dicalcium	-48.05	8.75	56.80	Ca2Fe2O5
Ferrite-Mg	-13.67	7.35	21.02	MgFe2O4
Ferrite-Zn	-5.67	6.03	11.70	ZnFe2O4
FeSO4	-8.10	-5.49	2.61	FeSO4
Gaylussite	-34.09	-22.93	11.16	CaNa2(CO3)2:5H2O
Gibbsite	-4.75	2.99	7.74	Al(OH)3
Glauberite	-9.47	-14.94	-5.47	Na2Ca(SO4)2
Goethite	2.48	3.01	0.53	FeOOH
Gypsum	-1.17	-5.70	-4.53	CaSO4:2H2O
H2(g)	-28.92	-32.02	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-8.19	-6.63	1.56	NaCl
Hausmannite	-30.96	-20.81	10.14	Mn3O4
HCl(g)	-11.85	-5.54	6.30	HCl
Hematite	5.95	6.03	0.08	Fe2O3
Hercynite	-21.26	7.55	28.80	FeAl2O4
Hexahydrite	-4.02	-5.74	-1.73	MgSO4:6H2O
Huntite	-49.12	-38.91	10.22	CaMg3(CO3)4
Hydromagnesite	-68.37	-37.63	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.47	-9.73	11.75	CaCl2
Hydrozincite	-52.38	-22.08	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	2.24	-7.17	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	-0.73	-6.18	-5.45	NaFe3(SO4)2(OH)6
K	-66.02	4.96	70.98	K
K(g)	-76.62	4.96	81.58	K
K2CO3:1.5H2O	-28.60	-15.23	13.38	K2CO3:1.5H2O
K2O	-88.20	-4.17	84.04	K2O
K3H(SO4)2	-16.76	-20.38	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-110.73	-83.02	27.71	K8H4(CO3)6:3H2O
Kainite	-13.06	-13.37	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-16.50	-13.22	3.27	KAl(SO4)2
Kalinite	-13.43	-13.14	0.28	KHCO3
Katoite	-68.88	10.07	78.94	Ca3Al2H12O12
Kieserite	-5.48	-5.74	-0.27	MgSO4:H2O
KMgCl3	-38.64	-17.39	21.25	KMgCl3
KMgCl3:2H2O	-31.36	-17.39	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-24.49	-14.23	10.26	KNaCO3:6H2O
Lammerite	-23.26	-21.71	1.55	Cu3(AsO4)2
Lansfordite	-14.58	-9.74	4.84	MgCO3:5H2O
Lawrencite	-18.57	-9.52	9.05	FeCl2
Leonite	-12.86	-16.97	-4.11	K2Mg(SO4)2:4H2O
Lime	-31.21	1.36	32.57	CaO
Magnesite	-12.01	-9.74	2.27	MgCO3
Magnetite	-2.82	7.60	10.42	Fe3O4
Malachite	-21.08	-15.18	5.90	Cu2CO3(OH)2
Manganite	-10.48	-10.64	-0.16	MnO(OH)
Manganosite	-17.44	0.47	17.92	MnO
Mayenite	-435.96	58.19	494.15	Ca12Al14O33

Melanterite	-3.10	-5.49	-2.40	FeSO4:7H2O
Mercallite	-7.71	-9.15	-1.44	KHSO4
Mg	-107.12	15.40	122.52	Mg
Mg(g)	-126.85	15.40	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.61	-5.41	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-14.29	-5.08	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.50	-9.77	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.07	-9.77	7.30	MgCl2:4H2O
MgCl2:H2O	-25.84	-9.77	16.07	MgCl2:H2O
MgOHCl	-20.11	-4.22	15.89	MgOHCl
MgSO4	-10.57	-5.74	4.83	MgSO4
Mirabilite	-8.08	-9.24	-1.15	Na2SO4:10H2O
Misenite	-55.04	-66.12	-11.08	K8H6(SO4)7
Mn	-68.38	14.55	82.93	Mn
Mn(OH)2(am)	-14.84	0.47	15.31	Mn(OH)2
Mn(OH)3	-16.98	-10.64	6.34	Mn(OH)3
MnCl2:2H2O	-14.61	-10.62	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.37	-10.62	2.75	MnCl2:4H2O
MnCl2:H2O	-16.16	-10.62	5.54	MnCl2:H2O
MnO2(gamma)	-13.71	-29.83	-16.13	MnO2
MnSO4	-9.20	-6.59	2.61	MnSO4
Molysite	-27.09	-13.62	13.47	FeCl3
Monohydrocalcite	-12.37	-9.70	2.68	CaCO3:H2O
Na	-61.42	5.95	67.37	Na
Na(g)	-74.91	5.95	80.86	Na
Na2CO3	-24.39	-13.23	11.16	Na2CO3
Na2CO3:7H2O	-23.17	-13.23	9.94	Na2CO3:7H2O
Na2O	-69.59	-2.17	67.42	Na2O
Na3H(SO4)2	-16.49	-17.38	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-18.28	-24.17	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-17.96	1.93	19.88	NaFeO2
Nahcolite	-12.00	-12.14	-0.14	NaHCO3
Nantokite	-12.56	-19.33	-6.77	CuCl
Natron	-22.82	-13.23	9.59	Na2CO3:10H2O
Nesquehonite	-15.03	-9.74	5.29	MgCO3:3H2O
Niter	-6.86	-7.09	-0.22	KNO3
NO2(g)	-6.32	2.03	8.35	NO2
O2(g)	-25.26	-28.16	-2.89	O2
Oxychloride-Mg	-28.73	-2.90	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.36	-5.74	-1.39	MgSO4:5H2O
Periclase	-20.00	1.32	21.33	MgO
Picromerite	-12.53	-16.97	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-34.25	-22.93	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-14.06	-28.38	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-21.18	1.36	22.55	Ca(OH)2
Pyrolusite	-12.17	-29.83	-17.66	MnO2
Rhodochrosite	-10.37	-10.59	-0.22	MnCO3
Scacchite	-19.36	-10.62	8.74	MnCl2
Siderite	-9.27	-9.49	-0.22	FeCO3
Smithsonite	-11.49	-11.05	0.44	ZnCO3
Spinel	-30.31	7.30	37.61	Al2MgO4
Starkeyite	-4.74	-5.74	-1.00	MgSO4:4H2O
Sylvite	-8.45	-7.63	0.83	KCl
Syngenite	-9.33	-16.93	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-46.40	-29.26	17.14	Mg2CaCl6:12H2O
Tenorite	-9.71	-2.06	7.65	CuO
Thenardite	-8.88	-9.23	-0.36	Na2SO4
Thermonatrite	-24.17	-13.23	10.94	Na2CO3:H2O
Todorokite	-78.16	-123.99	-45.82	Mn7O12:3H2O
Trona-K	-38.96	-27.37	11.59	K2NaH(CO3)2:2H2O
Wustite	-10.76	1.64	12.40	Fe.9470
Zincite	-11.19	0.01	11.20	ZnO
Zn	-54.70	14.09	68.79	Zn
Zn(ClO4)2:6H2O	-160.79	-155.15	5.63	Zn(ClO4)2:6H2O
Zn(g)	-71.32	14.09	85.41	Zn
Zn(NO3)2:6H2O	-13.40	-10.00	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-11.92	0.01	11.93	Zn(OH)2

Zn(OH)2(epsilon)	-11.65	0.01	11.66	Zn(OH)2
Zn(OH)2(gamma)	-11.87	0.01	11.88	Zn(OH)2
Zn2(OH)3Cl	-20.82	-5.53	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-14.63	-7.05	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-24.81	-15.49	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-33.19	-14.10	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-52.64	-9.97	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.16	-11.08	7.08	ZnCl2
ZnCO3:H2O	-11.19	-11.05	0.14	ZnCO3:H2O
ZnSO4	-10.59	-7.06	3.53	ZnSO4
ZnSO4:6H2O	-5.36	-7.06	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.18	-7.06	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.51	-7.06	-0.55	ZnSO4:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 1.

Mixture 1.

6.000e+000 Solution 1 UGA1
4.000e+000 Solution 2 UGA2

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

Elements	Molality	Moles
Al	3.120e-004	3.120e-003
As	3.719e-006	3.719e-005
C	8.018e-006	8.018e-005
Ca	8.720e-004	8.720e-003
Cl	1.278e-003	1.278e-002
Cu	1.379e-006	1.379e-005
Fe	7.768e-004	7.768e-003
K	4.040e-004	4.040e-003
Mg	4.738e-004	4.738e-003
Mn	1.094e-004	1.094e-003
N	3.538e-003	3.538e-002
Na	6.166e-004	6.166e-003
S	9.868e-003	9.868e-002
Zn	2.231e-005	2.231e-004

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

pH	=	2.805	Charge balance
pe	=	17.283	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	2.510e-002	
Mass of water (kg)	=	1.000e+001	
Total alkalinity (eq/kg)	=	-3.537e-003	
Total CO2 (mol/kg)	=	8.018e-006	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-1.521e-001	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-52.62	
Iterations	=	13	
Total H	=	1.110537e+003	
Total O	=	5.557563e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
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	H+	1.776e-003	1.568e-003	-2.751	-2.805	-0.054
	OH-	7.178e-012	6.144e-012	-11.144	-11.212	-0.067
	H2O	5.553e+001	9.997e-001	1.744	-0.000	0.000
Al	3.120e-004					
	AlSO4+	1.610e-004	1.383e-004	-3.793	-3.859	-0.066
	Al+3	9.503e-005	3.037e-005	-4.022	-4.518	-0.495
	Al(SO4)2-	5.559e-005	4.775e-005	-4.255	-4.321	-0.066
	AlOH+2	3.962e-007	2.170e-007	-6.402	-6.664	-0.262
	Al(OH)2+	3.741e-010	3.213e-010	-9.427	-9.493	-0.066
	Al2(OH)2+4	7.773e-011	7.656e-012	-10.109	-11.116	-1.007
	HALO2	2.983e-013	2.983e-013	-12.525	-12.525	0.000
	Al3(OH)4+5	2.127e-015	6.104e-017	-14.672	-16.214	-1.542
	AlO2-	7.589e-017	6.519e-017	-16.120	-16.186	-0.066
	NaAlO2	6.398e-021	6.398e-021	-20.194	-20.194	0.000
	Al13O4(OH)24+7	0.000e+000	0.000e+000	-64.685	-67.709	-3.024
As(-3)	0.000e+000					
	AsH3	0.000e+000	0.000e+000	-152.302	-152.302	0.000
As(3)	2.771e-027					
	HAsO2	1.479e-027	1.479e-027	-26.830	-26.830	0.000
	As(OH)3	1.292e-027	1.292e-027	-26.889	-26.889	0.000
	H2AsO3-	5.870e-034	5.042e-034	-33.231	-33.297	-0.066
	AsO2-	5.613e-034	4.822e-034	-33.251	-33.317	-0.066
	AsO2OH-2	0.000e+000	0.000e+000	-41.236	-41.503	-0.267
	HAsS2	0.000e+000	0.000e+000	-275.526	-275.526	0.000
As(5)	3.719e-006					
	H2AsO4-	3.005e-006	2.582e-006	-5.522	-5.588	-0.066
	H3AsO4	7.128e-007	7.128e-007	-6.147	-6.147	0.000
	HAsO4-2	5.058e-010	2.734e-010	-9.296	-9.563	-0.267
	AsO4-3	1.791e-018	4.474e-019	-17.747	-18.349	-0.602
C(-2)	0.000e+000					
	C2H4	0.000e+000	0.000e+000	-260.398	-260.398	0.000
C(-3)	0.000e+000					
	C2H6	0.000e+000	0.000e+000	-231.686	-231.686	0.000
C(-4)	0.000e+000					
	CH4	0.000e+000	0.000e+000	-144.259	-144.259	0.000
C(2)	0.000e+000					
	CO	0.000e+000	0.000e+000	-50.310	-50.310	0.000
C(4)	8.018e-006					
	CO2	8.015e-006	8.064e-006	-5.096	-5.093	0.003
	HCO3-	2.581e-009	2.217e-009	-8.588	-8.654	-0.066
	FeCO3+	2.551e-011	2.192e-011	-10.593	-10.659	-0.066
	CaHCO3+	1.098e-011	9.433e-012	-10.959	-11.025	-0.066
	MgHCO3+	4.935e-012	4.239e-012	-11.307	-11.373	-0.066
	NaHCO3	1.632e-012	1.632e-012	-11.787	-11.787	0.000
	MnHCO3+	7.498e-013	6.441e-013	-12.125	-12.191	-0.066
	ZnHCO3+	5.500e-013	4.725e-013	-12.260	-12.326	-0.066
	FeHCO3+	4.457e-015	3.828e-015	-14.351	-14.417	-0.066
	CuCO3	2.965e-016	2.965e-016	-15.528	-15.528	0.000
	CO3-2	1.146e-016	6.275e-017	-15.941	-16.202	-0.262
	MnCO3	8.381e-017	8.381e-017	-16.077	-16.077	0.000
	CaCO3	5.221e-017	5.221e-017	-16.282	-16.282	0.000
	MgCO3	1.093e-017	1.093e-017	-16.962	-16.962	0.000
	ZnCO3	4.356e-018	4.356e-018	-17.361	-17.361	0.000
	NaCO3-	1.315e-019	1.130e-019	-18.881	-18.947	-0.066
	FeCO3	1.172e-020	1.172e-020	-19.931	-19.931	0.000
	Cu(CO3)2-2	6.132e-029	3.315e-029	-28.212	-28.480	-0.267
	CuCO3(OH)2-2	1.897e-030	1.025e-030	-29.722	-29.989	-0.267
Ca	8.720e-004					
	Ca+2	6.324e-004	3.590e-004	-3.199	-3.445	-0.246
	CaSO4	2.333e-004	2.333e-004	-3.632	-3.632	0.000
	CaNO3+	6.101e-006	5.240e-006	-5.215	-5.281	-0.066
	CaCl+	9.651e-008	8.290e-008	-7.015	-7.081	-0.066
	CaCl2	1.062e-010	1.062e-010	-9.974	-9.974	0.000
	CaHCO3+	1.098e-011	9.433e-012	-10.959	-11.025	-0.066
	CaOH+	3.765e-014	3.234e-014	-13.424	-13.490	-0.066
	CaCO3	5.221e-017	5.221e-017	-16.282	-16.282	0.000
Cl(-1)	1.278e-003					

Cl-	1.277e-003	1.089e-003	-2.894	-2.963	-0.069
HCl	3.835e-007	3.835e-007	-6.416	-6.416	0.000
MgCl+	1.630e-007	1.400e-007	-6.788	-6.854	-0.066
MnCl+	1.030e-007	8.850e-008	-6.987	-7.053	-0.066
NaCl	9.850e-008	9.850e-008	-7.007	-7.007	0.000
CaCl+	9.651e-008	8.290e-008	-7.015	-7.081	-0.066
FeCl+2	2.004e-008	1.098e-008	-7.698	-7.960	-0.262
ZnCl+	1.761e-008	1.513e-008	-7.754	-7.820	-0.066
KCl	1.217e-008	1.217e-008	-7.915	-7.915	0.000
FeCl2+	1.127e-008	9.681e-009	-7.948	-8.014	-0.066
CuCl+	1.719e-009	1.476e-009	-8.765	-8.831	-0.066
CaCl2	1.062e-010	1.062e-010	-9.974	-9.974	0.000
ZnCl2	1.925e-011	1.925e-011	-10.715	-10.715	0.000
FeCl+	3.040e-012	2.611e-012	-11.517	-11.583	-0.066
CuCl2	8.469e-013	8.469e-013	-12.072	-12.072	0.000
Zn(OH)Cl	1.650e-013	1.650e-013	-12.783	-12.783	0.000
MnCl3-	2.671e-014	2.294e-014	-13.573	-13.639	-0.066
ZnCl3-	1.349e-014	1.158e-014	-13.870	-13.936	-0.066
ZnCl4-2	1.770e-016	9.565e-017	-15.752	-16.019	-0.267
FeCl4-	1.608e-017	1.381e-017	-16.794	-16.860	-0.066
FeCl2	1.526e-017	1.526e-017	-16.816	-16.816	0.000
CuCl2-	1.295e-022	1.112e-022	-21.888	-21.954	-0.066
FeCl4-2	9.684e-023	5.234e-023	-22.014	-22.281	-0.267
CuCl4-2	3.490e-023	1.886e-023	-22.457	-22.724	-0.267
CuCl3-2	1.440e-024	7.783e-025	-23.842	-24.109	-0.267
Cl(1)	7.375e-017				
HClO	7.375e-017	7.375e-017	-16.132	-16.132	0.000
ClO-	1.477e-021	1.269e-021	-20.831	-20.897	-0.066
Cl(3)	6.557e-032				
HClO2	4.364e-032	4.364e-032	-31.360	-31.360	0.000
ClO2-	2.192e-032	1.883e-032	-31.659	-31.725	-0.066
Cl(5)	2.324e-029				
ClO3-	2.324e-029	1.989e-029	-28.634	-28.701	-0.067
Cl(7)	1.225e-030				
ClO4-	1.225e-030	1.049e-030	-29.912	-29.979	-0.067
ZnClO4+	1.909e-034	1.640e-034	-33.719	-33.785	-0.066
Cu(1)	1.778e-021				
Cu+	1.647e-021	1.415e-021	-20.783	-20.849	-0.066
CuCl2-	1.295e-022	1.112e-022	-21.888	-21.954	-0.066
CuCl3-2	1.440e-024	7.783e-025	-23.842	-24.109	-0.267
Cu(2)	1.379e-006				
Cu+2	8.727e-007	4.955e-007	-6.059	-6.305	-0.246
CuSO4	5.050e-007	5.050e-007	-6.297	-6.297	0.000
CuCl+	1.719e-009	1.476e-009	-8.765	-8.831	-0.066
CuOH+	1.897e-011	1.630e-011	-10.722	-10.788	-0.066
CuCl2	8.469e-013	8.469e-013	-12.072	-12.072	0.000
CuCO3	2.965e-016	2.965e-016	-15.528	-15.528	0.000
CuNO2+	6.841e-020	5.876e-020	-19.165	-19.231	-0.066
CuCl4-2	3.490e-023	1.886e-023	-22.457	-22.724	-0.267
Cu(CO3)2-2	6.132e-029	3.315e-029	-28.212	-28.480	-0.267
CuCO3(OH)2-2	1.897e-030	1.025e-030	-29.722	-29.989	-0.267
Cu(NO2)2	6.811e-034	6.811e-034	-33.167	-33.167	0.000
CuO2-2	5.386e-035	2.912e-035	-34.269	-34.536	-0.267
CuNH3+2	0.000e+000	0.000e+000	-58.121	-58.382	-0.262
Cu(NH3)2+2	0.000e+000	0.000e+000	-110.804	-111.066	-0.262
Cu(NH3)3+2	0.000e+000	0.000e+000	-164.101	-164.362	-0.262
Fe(2)	8.118e-009				
Fe+2	5.796e-009	3.290e-009	-8.237	-8.483	-0.246
FeSO4	2.320e-009	2.320e-009	-8.635	-8.635	0.000
FeCl+	3.040e-012	2.611e-012	-11.517	-11.583	-0.066
FeHCO3+	4.457e-015	3.828e-015	-14.351	-14.417	-0.066
FeOH+	7.724e-016	6.635e-016	-15.112	-15.178	-0.066
FeCl2	1.526e-017	1.526e-017	-16.816	-16.816	0.000
FeCO3	1.172e-020	1.172e-020	-19.931	-19.931	0.000
FeCl4-2	9.684e-023	5.234e-023	-22.014	-22.281	-0.267
Fe(OH)2	3.361e-024	3.361e-024	-23.474	-23.474	0.000
Fe(OH)3-	9.934e-032	8.533e-032	-31.003	-31.069	-0.066

Fe(OH)4-2	0.000e+000	0.000e+000	-42.997	-43.264	-0.267
Fe(3)	7.768e-004				
FeOH+2	4.547e-004	2.490e-004	-3.342	-3.604	-0.262
Fe+3	1.892e-004	6.047e-005	-3.723	-4.218	-0.495
Fe(OH)2+	6.121e-005	5.258e-005	-4.213	-4.279	-0.066
FeSO4+	3.030e-005	2.603e-005	-4.519	-4.585	-0.066
Fe2(OH)2+4	1.694e-005	1.669e-006	-4.771	-5.778	-1.007
FeNO3+2	3.216e-006	1.761e-006	-5.493	-5.754	-0.262
Fe(SO4)2-	2.279e-006	1.958e-006	-5.642	-5.708	-0.066
Fe3(OH)4+5	6.388e-007	1.833e-008	-6.195	-7.737	-1.542
FeCl+2	2.004e-008	1.098e-008	-7.698	-7.960	-0.262
Fe(OH)3	1.568e-008	1.568e-008	-7.805	-7.805	0.000
FeCl2+	1.127e-008	9.681e-009	-7.948	-8.014	-0.066
FeCO3+	2.551e-011	2.192e-011	-10.593	-10.659	-0.066
Fe(OH)4-	2.925e-015	2.512e-015	-14.534	-14.600	-0.066
FeNO2+2	1.767e-016	9.675e-017	-15.753	-16.014	-0.262
FeCl4-	1.608e-017	1.381e-017	-16.794	-16.860	-0.066
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.278	-43.275	0.003
K	4.040e-004				
K+	3.900e-004	3.327e-004	-3.409	-3.478	-0.069
KSO4-	1.391e-005	1.195e-005	-4.857	-4.923	-0.066
KHSO4	1.652e-008	1.652e-008	-7.782	-7.782	0.000
KCl	1.217e-008	1.217e-008	-7.915	-7.915	0.000
KOH	7.357e-016	7.357e-016	-15.133	-15.133	0.000
Mg	4.738e-004				
Mg+2	2.781e-004	1.646e-004	-3.556	-3.784	-0.228
MgSO4	1.956e-004	1.956e-004	-3.709	-3.709	0.000
MgCl+	1.630e-007	1.400e-007	-6.788	-6.854	-0.066
MgHCO3+	4.935e-012	4.239e-012	-11.307	-11.373	-0.066
MgCO3	1.093e-017	1.093e-017	-16.962	-16.962	0.000
Mg4(OH)4+4	0.000e+000	0.000e+000	-42.659	-43.666	-1.007
Mn(2)	1.094e-004				
Mn+2	6.721e-005	3.815e-005	-4.173	-4.418	-0.246
MnSO4	4.188e-005	4.188e-005	-4.378	-4.378	0.000
MnNO3+	2.050e-007	1.761e-007	-6.688	-6.754	-0.066
MnCl+	1.030e-007	8.850e-008	-6.987	-7.053	-0.066
Mn(NO3)2	1.288e-009	1.288e-009	-8.890	-8.890	0.000
MnHCO3+	7.498e-013	6.441e-013	-12.125	-12.191	-0.066
MnOH+	7.281e-013	6.254e-013	-12.138	-12.204	-0.066
MnCl3-	2.671e-014	2.294e-014	-13.573	-13.639	-0.066
Mn2OH+3	9.665e-017	2.557e-017	-16.015	-16.592	-0.577
MnCO3	8.381e-017	8.381e-017	-16.077	-16.077	0.000
Mn(OH)2	9.791e-022	9.791e-022	-21.009	-21.009	0.000
Mn2(OH)3+	5.533e-025	4.753e-025	-24.257	-24.323	-0.066
Mn(OH)3-	6.818e-031	5.857e-031	-30.166	-30.232	-0.066
Mn(OH)4-2	0.000e+000	0.000e+000	-41.233	-41.500	-0.267
Mn(3)	7.374e-013				
Mn+3	7.374e-013	1.951e-013	-12.132	-12.710	-0.577
Mn(6)	9.331e-032				
MnO4-2	9.331e-032	5.044e-032	-31.030	-31.297	-0.267
Mn(7)	4.973e-024				
MnO4-	4.973e-024	4.258e-024	-23.303	-23.371	-0.067
N(-03)	0.000e+000				
HN3	0.000e+000	0.000e+000	-77.994	-77.994	0.000
N3-	0.000e+000	0.000e+000	-79.825	-79.891	-0.066
ZnN3+	0.000e+000	0.000e+000	-84.466	-84.532	-0.066
Zn(N3)2	0.000e+000	0.000e+000	-163.670	-163.670	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-49.611	-49.682	-0.071
NH3	0.000e+000	0.000e+000	-56.117	-56.117	0.000
CuNH3+2	0.000e+000	0.000e+000	-58.121	-58.382	-0.262
Zn(NH3)+2	0.000e+000	0.000e+000	-58.886	-59.147	-0.262
NH4SO4-	0.000e+000	0.000e+000	-60.268	-60.334	-0.066
Cu(NH3)2+2	0.000e+000	0.000e+000	-110.804	-111.066	-0.262
Zn(NH3)2+2	0.000e+000	0.000e+000	-112.796	-113.058	-0.262
Cu(NH3)3+2	0.000e+000	0.000e+000	-164.101	-164.362	-0.262

Zn(NH3)3+2	0.000e+000	0.000e+000	-166.707	-166.969	-0.262
Zn(NH3)4+2	0.000e+000	0.000e+000	-220.892	-221.154	-0.262
N(0)	1.140e-004				
N2	5.702e-005	5.702e-005	-4.244	-4.244	0.000
N(3)	4.535e-015				
HNO2	3.030e-015	3.030e-015	-14.519	-14.519	0.000
NO2-	1.328e-015	1.133e-015	-14.877	-14.946	-0.069
FeNO2+2	1.767e-016	9.675e-017	-15.753	-16.014	-0.262
CuNO2+	6.841e-020	5.876e-020	-19.165	-19.231	-0.066
Cu(NO2)2	6.811e-034	6.811e-034	-33.167	-33.167	0.000
N(5)	3.424e-003				
NO3-	3.414e-003	2.912e-003	-2.467	-2.536	-0.069
CaNO3+	6.101e-006	5.240e-006	-5.215	-5.281	-0.066
FeNO3+2	3.216e-006	1.761e-006	-5.493	-5.754	-0.262
HNO3	2.388e-007	2.388e-007	-6.622	-6.622	0.000
MnNO3+	2.050e-007	1.761e-007	-6.688	-6.754	-0.066
Mn(NO3)2	1.288e-009	1.288e-009	-8.890	-8.890	0.000
Na	6.166e-004				
Na+	5.989e-004	5.145e-004	-3.223	-3.289	-0.066
NaSO4-	1.760e-005	1.512e-005	-4.754	-4.820	-0.066
NaCl	9.850e-008	9.850e-008	-7.007	-7.007	0.000
NaHCO3	1.632e-012	1.632e-012	-11.787	-11.787	0.000
NaOH	5.454e-016	5.454e-016	-15.263	-15.263	0.000
NaCO3-	1.315e-019	1.130e-019	-18.881	-18.947	-0.066
NaAlO2	6.398e-021	6.398e-021	-20.194	-20.194	0.000
O(0)	4.494e-006				
O2	2.247e-006	2.261e-006	-5.648	-5.646	0.003
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-127.943	-127.943	0.000
HS-	0.000e+000	0.000e+000	-132.080	-132.148	-0.067
S-2	0.000e+000	0.000e+000	-142.013	-142.269	-0.256
S2-2	0.000e+000	0.000e+000	-233.593	-233.860	-0.267
HAsS2	0.000e+000	0.000e+000	-275.526	-275.526	0.000
S3-2	0.000e+000	0.000e+000	-325.226	-325.493	-0.267
S4-2	0.000e+000	0.000e+000	-417.086	-417.353	-0.267
S5-2	0.000e+000	0.000e+000	-509.162	-509.430	-0.267
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-132.228	-132.495	-0.267
HS2O3-	0.000e+000	0.000e+000	-134.220	-134.286	-0.066
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-119.990	-120.246	-0.256
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-41.654	-41.720	-0.066
H2SO3	0.000e+000	0.000e+000	-42.543	-42.543	0.000
SO2	0.000e+000	0.000e+000	-42.643	-42.643	0.000
SO3-2	0.000e+000	0.000e+000	-45.885	-46.147	-0.262
S2O6-2	0.000e+000	0.000e+000	-58.592	-58.859	-0.267
S3O6-2	0.000e+000	0.000e+000	-152.707	-152.974	-0.267
S4O6-2	0.000e+000	0.000e+000	-230.917	-231.184	-0.267
S5O6-2	0.000e+000	0.000e+000	-338.006	-338.274	-0.267
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-88.003	-88.270	-0.267
S(6)	9.868e-003				
SO4-2	8.230e-003	4.449e-003	-2.085	-2.352	-0.267
HSO4-	8.201e-004	7.045e-004	-3.086	-3.152	-0.066
CaSO4	2.333e-004	2.333e-004	-3.632	-3.632	0.000
MgSO4	1.956e-004	1.956e-004	-3.709	-3.709	0.000
AlSO4+	1.610e-004	1.383e-004	-3.793	-3.859	-0.066
Al(SO4)2-	5.559e-005	4.775e-005	-4.255	-4.321	-0.066
MnSO4	4.188e-005	4.188e-005	-4.378	-4.378	0.000
FeSO4+	3.030e-005	2.603e-005	-4.519	-4.585	-0.066
NaSO4-	1.760e-005	1.512e-005	-4.754	-4.820	-0.066
KSO4-	1.391e-005	1.195e-005	-4.857	-4.923	-0.066
ZnSO4	7.728e-006	7.728e-006	-5.112	-5.112	0.000
Fe(SO4)2-	2.279e-006	1.958e-006	-5.642	-5.708	-0.066
CuSO4	5.050e-007	5.050e-007	-6.297	-6.297	0.000
KHSO4	1.652e-008	1.652e-008	-7.782	-7.782	0.000

FeSO4	2.320e-009	2.320e-009	-8.635	-8.635	0.000
H2SO4	1.042e-009	1.042e-009	-8.982	-8.982	0.000
NH4SO4-	0.000e+000	0.000e+000	-60.268	-60.334	-0.066
S(7)	9.491e-036				
S2O8-2	4.746e-036	2.565e-036	-35.324	-35.591	-0.267
S(8)	6.698e-026				
HSO5-	6.698e-026	5.754e-026	-25.174	-25.240	-0.066
Zn	2.231e-005				
Zn+2	1.456e-005	8.267e-006	-4.837	-5.083	-0.246
ZnSO4	7.728e-006	7.728e-006	-5.112	-5.112	0.000
ZnCl+	1.761e-008	1.513e-008	-7.754	-7.820	-0.066
ZnCl2	1.925e-011	1.925e-011	-10.715	-10.715	0.000
ZnOH+	6.731e-012	5.782e-012	-11.172	-11.238	-0.066
ZnHCO3+	5.500e-013	4.725e-013	-12.260	-12.326	-0.066
Zn(OH)Cl	1.650e-013	1.650e-013	-12.783	-12.783	0.000
ZnCl3-	1.349e-014	1.158e-014	-13.870	-13.936	-0.066
ZnCl4-2	1.770e-016	9.565e-017	-15.752	-16.019	-0.267
Zn(OH)2	1.579e-017	1.579e-017	-16.802	-16.802	0.000
ZnCO3	4.356e-018	4.356e-018	-17.361	-17.361	0.000
Zn(OH)3-	3.634e-026	3.121e-026	-25.440	-25.506	-0.066
ZnClO4+	1.909e-034	1.640e-034	-33.719	-33.785	-0.066
Zn(OH)4-2	6.278e-036	3.394e-036	-35.202	-35.469	-0.267
Zn(NH3)+2	0.000e+000	0.000e+000	-58.886	-59.147	-0.262
ZnN3+	0.000e+000	0.000e+000	-84.466	-84.532	-0.066
Zn(NH3)2+2	0.000e+000	0.000e+000	-112.796	-113.058	-0.262
Zn(N3)2	0.000e+000	0.000e+000	-163.670	-163.670	0.000
Zn(NH3)3+2	0.000e+000	0.000e+000	-166.707	-166.969	-0.262
Zn(NH3)4+2	0.000e+000	0.000e+000	-220.892	-221.154	-0.262

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

Phase	SI	log IAP	log KT	
Al	-141.78	8.13	149.91	Al
Al(g)	-192.49	8.13	200.62	Al
Al2(SO4)3	-34.99	-16.09	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-17.65	-16.09	1.56	Al2(SO4)3:6H2O
Alabandite	-133.34	-133.76	-0.42	MnS
Alum-K	-7.73	-12.70	-4.97	KAl(SO4)2:12H2O
Alunite	-4.44	-4.91	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.45	-5.80	-4.35	CaSO4
Antarcticite	-13.46	-9.37	4.09	CaCl2:6H2O
Antlerite	-18.78	-10.05	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.54	-18.43	-3.89	NaK3(SO4)2
Aragonite	-11.26	-9.29	1.97	CaCO3
Arcanite	-7.46	-9.31	-1.84	K2SO4
Arsenolite	-52.36	-72.20	-19.84	As2O3
Arsenopyrite	-217.58	-232.03	-14.45	FeAsS
Artinite	-27.43	-7.81	19.63	Mg2CO3(OH)2:3H2O
As	-74.55	-31.87	42.68	As
As2O5	-18.92	-16.79	2.14	As2O5
As4O6(cubi)	-104.58	-144.41	-39.82	As4O6
As4O6(mono)	-104.36	-144.41	-40.05	As4O6
Atacamite	-28.58	-14.32	14.26	Cu4Cl2(OH)6
Azurite	-34.12	-25.00	9.12	Cu3(CO3)2(OH)2
Bassanite	-2.09	-5.80	-3.71	CaSO4:0.5H2O
Birnessite	-19.22	-104.77	-85.55	Mn8O14:5H2O
Bischofite	-14.10	-9.71	4.39	MgCl2:6H2O
Bixbyite	-7.63	-8.59	-0.96	Mn2O3
Bloedite	-12.59	-15.06	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-3.65	3.90	7.55	AlO2H
Bornite	-513.02	-615.56	-102.53	Cu5FeS4
Brochantite	-26.17	-10.74	15.42	Cu4(SO4)(OH)6
Brucite	-14.46	1.83	16.28	Mg(OH)2
Burkeite	-39.77	-30.28	9.49	Na6CO3(SO4)2
C	-69.96	-5.81	64.15	C
C(g)	-187.58	-5.81	181.77	C

Ca	-134.84	4.99	139.83	Ca
Ca(g)	-160.08	4.99	165.07	Ca
Ca2Al2O5:8H2O	-47.45	12.12	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-33.50	-7.21	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-28.09	-10.29	17.80	Ca3(AsO4)2
Ca3Al2O6	-98.74	14.29	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-115.64	24.84	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-90.80	16.45	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-87.23	16.45	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-71.21	-2.88	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-36.95	9.96	46.91	CaAl2O4
CaAl2O4:10H2O	-28.04	9.96	37.99	CaAl2O4:10H2O
CaAl4O7	-50.84	17.75	68.59	CaAl4O7
Calcite	-11.12	-9.29	1.82	CaCO3
Carnallite	-20.42	-16.15	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.26	-5.80	-3.54	CaSO4:0.5H2O
CH4(g)	-141.42	-144.26	-2.84	CH4
Chalcanthite	-6.03	-8.66	-2.63	CuSO4:5H2O
Chalcocite	-136.30	-171.04	-34.74	Cu2S
Chalcocyanite	-11.57	-8.66	2.91	CuSO4
Chalcopyrite	-240.87	-273.47	-32.60	CuFeS2
Chloromagnesite	-31.52	-9.71	21.82	MgCl2
Cl2(g)	-17.35	-14.36	2.99	Cl2
Claudetite	-52.41	-72.20	-19.80	As2O3
CO(g)	-47.31	-50.31	-3.00	CO
CO2(g)	-3.63	-11.46	-7.83	CO2
Corundum	-10.50	7.79	18.29	Al2O3
Covellite	-112.79	-135.65	-22.86	CuS
Cu	-29.37	2.13	31.50	Cu
Cu(g)	-81.53	2.13	83.66	Cu
CuCl2	-15.95	-12.23	3.72	CuCl2
Cuprite	-34.18	-36.09	-1.91	Cu2O
Dawsonite	-12.39	-8.05	4.34	NaAlCO3(OH)2
Delafoosite	-7.41	-13.85	-6.44	CuFeO2
Diaspore	-3.25	3.90	7.15	AlHO2
Dolomite	-21.40	-18.93	2.47	CaMg(CO3)2
Dolomite-dis	-22.94	-18.93	4.01	CaMg(CO3)2
Dolomite-ord	-21.39	-18.93	2.46	CaMg(CO3)2
Epsomite	-4.17	-6.14	-1.96	MgSO4:7H2O
Ettringite	-65.57	-3.11	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-59.07	-0.05	59.02	Fe
Fe(OH)2	-16.77	-2.87	13.89	Fe(OH)2
Fe(OH)3	-1.44	4.20	5.64	Fe(OH)3
Fe2(SO4)3	-18.54	-15.49	3.05	Fe2(SO4)3
FeO	-16.40	-2.87	13.52	FeO
Ferrite-Ca	-10.94	10.56	21.50	CaFe2O4
Ferrite-Cu	-2.59	7.70	10.28	CuFe2O4
Ferrite-Dicalcium	-44.08	12.72	56.80	Ca2Fe2O5
Ferrite-Mg	-10.80	10.22	21.02	MgFe2O4
Ferrite-Zn	-2.78	8.92	11.70	ZnFe2O4
FeSO4	-13.44	-10.83	2.61	FeSO4
Gaylussite	-32.89	-21.72	11.16	CaNa2(CO3)2:5H2O
Gibbsite	-3.84	3.90	7.74	Al(OH)3
Glauberite	-9.26	-14.73	-5.47	Na2Ca(SO4)2
Goethite	3.67	4.20	0.53	FeOOH
Gypsum	-1.27	-5.80	-4.53	CaSO4:2H2O
H2(g)	-40.17	-43.28	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-126.96	-134.95	-7.99	H2S
Halite	-7.81	-6.25	1.56	NaCl
Hausmannite	-17.54	-7.40	10.14	Mn3O4
HCl(g)	-12.07	-5.77	6.30	HCl
Hematite	8.32	8.39	0.08	Fe2O3
Hercynite	-23.88	4.92	28.80	FeAl2O4
Hexahydrate	-4.41	-6.14	-1.73	MgSO4:6H2O
Huntite	-48.41	-38.19	10.22	CaMg3(CO3)4
Hydromagnesite	-67.45	-36.71	30.74	Mg5(CO3)4(OH)2:4H2O

Hydrophilite	-21.12	-9.37	11.75	CaCl ₂
Hydrozincite	-50.59	-20.28	30.31	Zn ₅ (OH) ₆ (CO ₃) ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Jarosite	5.40	-4.01	-9.41	KFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-Na	1.63	-3.82	-5.45	NaFe ₃ (SO ₄) ₂ (OH) ₆
K	-70.24	0.74	70.98	K
K(g)	-80.84	0.74	81.58	K
K ₂ CO ₃ :1.5H ₂ O	-26.18	-12.81	13.38	K ₂ CO ₃ :1.5H ₂ O
K ₂ O	-85.38	-1.35	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-14.32	-17.94	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ :3H ₂ O	-101.85	-74.14	27.71	K ₈ H ₄ (CO ₃) ₆ :3H ₂ O
Kainite	-12.27	-12.58	-0.31	KMgClSO ₄ :3H ₂ O
KAl(SO ₄) ₂	-15.97	-12.70	3.27	KAl(SO ₄) ₂
Kalicinite	-12.42	-12.13	0.28	KHCO ₃
Katoite	-64.66	14.29	78.94	Ca ₃ Al ₂ H ₁₂ O ₁₂
Kieserite	-5.87	-6.14	-0.27	MgSO ₄ :H ₂ O
KMgCl ₃	-37.40	-16.15	21.25	KMgCl ₃
KMgCl ₃ :2H ₂ O	-30.11	-16.15	13.96	KMgCl ₃ :2H ₂ O
KNaCO ₃ :6H ₂ O	-22.88	-12.62	10.26	KNaCO ₃ :6H ₂ O
Lammerite	-20.43	-18.87	1.55	Cu ₃ (AsO ₄) ₂
Lansfordite	-14.47	-9.63	4.84	MgCO ₃ :5H ₂ O
Lawrencite	-23.46	-14.41	9.05	FeCl ₂
Leonite	-11.33	-15.44	-4.11	K ₂ Mg(SO ₄) ₂ :4H ₂ O
Lime	-30.40	2.16	32.57	CaO
Magnesite	-11.91	-9.63	2.27	MgCO ₃
Magnetite	-4.90	5.52	10.42	Fe ₃ O ₄
Malachite	-18.75	-12.85	5.90	Cu ₂ CO ₃ (OH) ₂
Manganite	-4.13	-4.30	-0.16	MnO(OH)
Manganosite	-16.73	1.19	17.92	MnO
Mayenite	-413.62	80.53	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-8.44	-10.84	-2.40	FeSO ₄ :7H ₂ O
Mercallite	-7.20	-8.63	-1.44	KHSO ₄
Mg	-117.87	4.65	122.52	Mg
Mg(g)	-137.60	4.65	142.25	Mg
Mg ₁ .25SO ₄ (OH)0.5:0.5H ₂ O	-10.87	-5.68	5.20	Mg ₁ .25SO ₄ (OH)0.5:0.5H ₂ O
Mg ₁ .5SO ₄ (OH)	-14.43	-5.22	9.21	Mg ₁ .5SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.44	-9.71	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-17.01	-9.71	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-25.78	-9.71	16.07	MgCl ₂ :H ₂ O
MgOHCl	-19.83	-3.94	15.89	MgOHCl
MgSO ₄	-10.96	-6.14	4.83	MgSO ₄
Mirabilite	-7.78	-8.93	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-50.04	-61.11	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-78.92	4.01	82.93	Mn
Mn(OH) ₂ (am)	-14.12	1.19	15.31	Mn(OH) ₂
Mn(OH) ₃	-10.64	-4.30	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-14.34	-10.34	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-13.10	-10.34	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-15.89	-10.34	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-1.73	-17.86	-16.13	MnO ₂
MnSO ₄	-9.38	-6.77	2.61	MnSO ₄
Molysite	-26.58	-13.11	13.47	FeCl ₃
Monohydrocalcite	-11.97	-9.29	2.68	CaCO ₃ :H ₂ O
N ₂ (g)	-1.07	-4.24	-3.18	N ₂
Na	-66.44	0.93	67.37	Na
Na(g)	-79.93	0.93	80.86	Na
Na ₂ CO ₃	-23.59	-12.43	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-22.37	-12.43	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-68.39	-0.97	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-16.48	-17.37	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-17.76	-23.65	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-16.17	3.71	19.88	NaFeO ₂
Nahcolite	-11.80	-11.94	-0.14	NaHCO ₃
Nantokite	-17.05	-23.81	-6.77	CuCl
Natron	-22.02	-12.43	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-14.92	-9.63	5.29	MgCO ₃ :3H ₂ O
NH ₃ (g)	-57.91	-56.12	1.80	NH ₃

Niter	-5.79	-6.01	-0.22	KNO3
NO(g)	-17.08	-16.34	0.74	NO
NO2(g)	-12.28	-3.93	8.35	NO2
O2(g)	-2.75	-5.65	-2.89	O2
Orpiment	-397.58	-477.06	-79.49	As2S3
Oxychloride-Mg	-27.95	-2.12	25.83	Mg2Cl(OH)3:4H2O
Pentahydrite	-4.75	-6.14	-1.39	MgSO4:5H2O
Periclase	-19.50	1.83	21.33	MgO
Picromerite	-11.00	-15.44	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-33.04	-21.72	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-12.72	-27.04	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-20.38	2.16	22.55	Ca(OH)2
Pyrite	-216.33	-241.03	-24.70	FeS2
Pyrolusite	-0.20	-17.86	-17.66	MnO2
Pyrrhotite	-134.09	-137.83	-3.74	FeS
Realgar	-154.95	-215.23	-60.28	AsS
Rhodochrosite	-10.05	-10.27	-0.22	MnCO3
S	-92.66	-137.78	-45.11	S
S2(g)	-199.22	-206.41	-7.19	S2
Scacchite	-19.09	-10.34	8.74	MnCl2
Siderite	-14.11	-14.33	-0.22	FeCO3
Smithsonite	-11.38	-10.93	0.44	ZnCO3
SO2(g)	-42.82	-42.64	0.18	SO2
Sphalerite	-122.96	-134.43	-11.47	ZnS
Spinel	-27.99	9.62	37.61	Al2MgO4
Starkeyite	-5.14	-6.14	-1.00	MgSO4:4H2O
Sylvite	-7.27	-6.44	0.83	KCl
Syngenite	-7.50	-15.10	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.93	-28.79	17.14	Mg2CaCl6:12H2O
Tenorite	-8.34	-0.70	7.65	CuO
Thenardite	-8.57	-8.93	-0.36	Na2SO4
Thermonatrite	-23.36	-12.43	10.94	Na2CO3:H2O
Todorokite	-16.86	-62.68	-45.82	Mn7O12:3H2O
Troilite	-133.98	-137.83	-3.84	FeS
Trona-K	-36.34	-24.75	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-125.26	-134.43	-9.17	ZnS
Wustite	-14.37	-1.97	12.40	Fe.947O
Zincite	-10.67	0.53	11.20	ZnO
Zn	-65.44	3.35	68.79	Zn
Zn(ClO4)2:6H2O	-70.68	-65.04	5.63	Zn(ClO4)2:6H2O
Zn(g)	-82.06	3.35	85.41	Zn
Zn(NO3)2:6H2O	-13.56	-10.16	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-11.41	0.53	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-11.13	0.53	11.66	Zn(OH)2
Zn(OH)2(gamma)	-11.36	0.53	11.88	Zn(OH)2
Zn2(OH)3Cl	-20.01	-4.71	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-14.49	-6.91	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-24.52	-15.21	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-33.43	-14.34	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-50.72	-8.05	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.09	-11.01	7.08	ZnCl2
ZnCl2(NH3)2	-116.24	-123.24	-7.01	ZnCl2(NH3)2
ZnCl2(NH3)4	-228.77	-235.48	-6.71	ZnCl2(NH3)4
ZnCl2(NH3)6	-342.97	-347.71	-4.74	ZnCl2(NH3)6
ZnCO3:H2O	-11.07	-10.93	0.14	ZnCO3:H2O
ZnSO4	-10.97	-7.43	3.53	ZnSO4
ZnSO4:6H2O	-5.74	-7.44	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.56	-7.44	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.88	-7.43	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
