

Appendix 8.E

**PHREEQC thermodynamic equilibrium results
from water analyses in the test cells**

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

SOLUTION 1 Cell 1B
temp 17.4
pH 11.79
pe 4.0
redox pe
units mg/l
density 1:0
Al 1.10
B 0.24
Ba 0.31
Br 2.7
C(4) 1279 charge
Ca 810
Cl 70
Cu 0.02
F 4.3
K 410
Mg 0.07
N(5) 21.9
Na 130
P .000000316 Mol/l
Pb 0.01
S(6) 1600
Si 5.8
Sr 5.0

Beginning of initial solution calculations.

Initial solution 1. Cell 1B

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

Elements	Molality	Moles	
Al	4.095e-05	4.095e-05	
B	2.230e-05	2.230e-05	
Ba	2.267e-06	2.267e-06	
Br	3.394e-05	3.394e-05	
C(4)	7.352e-03	7.352e-03	Charge balance
Ca	2.030e-02	2.030e-02	

Cl	1.983e-03	1.983e-03
Cu	3.161e-07	3.161e-07
F	2.273e-04	2.273e-04
K	1.053e-02	1.053e-02
Mg	2.892e-06	2.892e-06
N(5)	1.570e-03	1.570e-03
Na	5.679e-03	5.679e-03
P	3.174e-07	3.174e-07
Pb	4.848e-08	4.848e-08
S(6)	1.673e-02	1.673e-02
Si	9.695e-05	9.695e-05
Sr	5.731e-05	5.731e-05

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

pH	=	11.790
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	5.988e-02
Mass of water (kg)	=	1.000e+00
Total alkalinity (eq/kg)	=	1.978e-02
Total CO2 (mol/kg)	=	7.352e-03
Temperature (deg C)	=	17.400
Electrical balance (eq)	=	-5.950e-16
Iterations	=	9
Total H	=	1.110178e+02
Total O	=	5.560535e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	4.229e-03	3.389e-03	-2.374	-2.470	-0.096
H+	1.912e-12	1.622e-12	-11.718	-11.790	-0.072
H2O	5.551e+01	9.990e-01	0.000	0.000	0.000
Al	4.095e-05				
Al(OH)4-	4.095e-05	3.329e-05	-4.388	-4.478	-0.090
Al(OH)3	3.084e-11	3.127e-11	-10.511	-10.505	0.006
Al(OH)2+	7.636e-16	6.209e-16	-15.117	-15.207	-0.090
AlOH+2	5.892e-22	2.575e-22	-21.230	-21.589	-0.359
AlF3	2.150e-23	2.180e-23	-22.668	-22.662	0.006
AlF2+	1.219e-23	9.909e-24	-22.914	-23.004	-0.090
AlF4-	1.876e-24	1.525e-24	-23.727	-23.817	-0.090
AlF+2	2.675e-25	1.169e-25	-24.573	-24.932	-0.359
AlF5-2	9.897e-27	4.326e-27	-26.005	-26.364	-0.359
AlSO4+	1.287e-27	1.047e-27	-26.890	-26.980	-0.090
Al+3	3.064e-28	6.957e-29	-27.514	-28.158	-0.644
Al(SO4)2-	2.066e-28	1.680e-28	-27.685	-27.775	-0.090
AlF6-3	5.726e-30	8.895e-31	-29.242	-30.051	-0.809
AlHSO4+2	3.244e-40	1.418e-40	-39.489	-39.848	-0.359
B	2.230e-05				
H2BO3-	2.224e-05	1.808e-05	-4.653	-4.743	-0.090
H3BO3	5.796e-08	5.876e-08	-7.237	-7.231	0.006
BF(OH)3-	4.670e-12	3.797e-12	-11.331	-11.421	-0.090
BF2(OH)2-	1.445e-19	1.175e-19	-18.840	-18.930	-0.090
BF3OH-	5.226e-29	4.249e-29	-28.282	-28.372	-0.090

	BF4-	6.149e-38	5.000e-38	-37.211	-37.301	-0.090
Ba		2.267e-06				
	BaSO4	1.127e-06	1.142e-06	-5.948	-5.942	0.006
	Ba+2	9.730e-07	4.330e-07	-6.012	-6.364	-0.352
	BaCO3	1.562e-07	1.583e-07	-6.806	-6.800	0.006
	BaOH+	1.112e-08	9.038e-09	-7.954	-8.044	-0.090
	BaHCO3+	1.357e-10	1.103e-10	-9.867	-9.957	-0.090
Br		3.394e-05				
	Br-	3.394e-05	2.700e-05	-4.469	-4.569	-0.099
C(4)		7.352e-03				
	CaCO3	5.425e-03	5.501e-03	-2.266	-2.260	0.006
	CO3-2	1.820e-03	8.245e-04	-2.740	-3.084	-0.344
	NaCO3-	5.678e-05	4.617e-05	-4.246	-4.336	-0.090
	HCO3-	4.115e-05	3.376e-05	-4.386	-4.472	-0.086
	SrCO3	6.675e-06	6.768e-06	-5.176	-5.170	0.006
	CaHCO3+	2.072e-06	1.700e-06	-5.684	-5.770	-0.086
	MgCO3	3.843e-07	3.896e-07	-6.415	-6.409	0.006
	BaCO3	1.562e-07	1.583e-07	-6.806	-6.800	0.006
	NaHCO3	8.345e-08	8.461e-08	-7.079	-7.073	0.006
	SrHCO3+	7.810e-09	6.408e-09	-8.107	-8.193	-0.086
	MgHCO3+	2.630e-10	2.139e-10	-9.580	-9.670	-0.090
	CO2	1.359e-10	1.377e-10	-9.867	-9.861	0.006
	BaHCO3+	1.357e-10	1.103e-10	-9.867	-9.957	-0.090
	Pb(CO3) 2-2	3.513e-11	1.535e-11	-10.454	-10.814	-0.359
	PbCO3	7.312e-12	7.413e-12	-11.136	-11.130	0.006
	PbHCO3+	1.707e-17	1.388e-17	-16.768	-16.858	-0.090
Ca		2.030e-02				
	Ca+2	9.937e-03	4.524e-03	-2.003	-2.344	-0.342
	CaCO3	5.425e-03	5.501e-03	-2.266	-2.260	0.006
	CaSO4	4.357e-03	4.417e-03	-2.361	-2.355	0.006
	CaOH+	5.688e-04	4.625e-04	-3.245	-3.335	-0.090
	CaF+	7.115e-06	5.785e-06	-5.148	-5.238	-0.090
	CaHCO3+	2.072e-06	1.700e-06	-5.684	-5.770	-0.086
	CaPO4-	3.167e-07	2.575e-07	-6.499	-6.589	-0.090
	CaHPO4	2.017e-10	2.045e-10	-9.695	-9.689	0.006
	CaHSO4+	4.728e-14	3.845e-14	-13.325	-13.415	-0.090
	CaH2PO4+	3.189e-16	2.593e-16	-15.496	-15.586	-0.090
Cl		1.983e-03				
	Cl-	1.983e-03	1.593e-03	-2.703	-2.798	-0.095
	PbCl+	3.325e-17	2.704e-17	-16.478	-16.568	-0.090
	PbCl2	7.786e-20	7.894e-20	-19.109	-19.103	0.006
	PbCl3-	1.170e-22	9.516e-23	-21.932	-22.022	-0.090
	PbCl4-2	1.563e-25	6.831e-26	-24.806	-25.166	-0.359
Cu(1)		2.364e-18				
	Cu+	2.364e-18	1.867e-18	-17.626	-17.729	-0.103
Cu(2)		3.161e-07				
	Cu(OH) 2	2.991e-07	3.032e-07	-6.524	-6.518	0.006
	Cu(OH) 3-	1.384e-08	1.126e-08	-7.859	-7.949	-0.090
	Cu(OH) 4-2	3.165e-09	1.383e-09	-8.500	-8.859	-0.359
	CuOH+	2.921e-13	2.356e-13	-12.535	-12.628	-0.093
	Cu+2	8.228e-17	3.825e-17	-16.085	-16.417	-0.333
	CuSO4	3.842e-17	3.895e-17	-16.415	-16.409	0.006
F		2.273e-04				
	F-	2.198e-04	1.761e-04	-3.658	-3.754	-0.096
	CaF+	7.115e-06	5.785e-06	-5.148	-5.238	-0.090
	NaF	4.454e-07	4.516e-07	-6.351	-6.345	0.006
	MgF+	6.914e-09	5.622e-09	-8.160	-8.250	-0.090

	BF(OH)3-	4.670e-12	3.797e-12	-11.331	-11.421	-0.090
	HF	3.693e-13	3.744e-13	-12.433	-12.427	0.006
	HF2-	2.912e-16	2.368e-16	-15.536	-15.626	-0.090
	BF2(OH)2-	1.445e-19	1.175e-19	-18.840	-18.930	-0.090
	AlF3	2.150e-23	2.180e-23	-22.668	-22.662	0.006
	AlF2+	1.219e-23	9.909e-24	-22.914	-23.004	-0.090
	AlF4-	1.876e-24	1.525e-24	-23.727	-23.817	-0.090
	AlF+2	2.675e-25	1.169e-25	-24.573	-24.932	-0.359
	AlF5-2	9.897e-27	4.326e-27	-26.005	-26.364	-0.359
	BF3OH-	5.226e-29	4.249e-29	-28.282	-28.372	-0.090
	AlF6-3	5.726e-30	8.895e-31	-29.242	-30.051	-0.809
	BF4-	6.149e-38	5.000e-38	-37.211	-37.301	-0.090
	SiF6-2	0.000e+00	0.000e+00	-44.798	-45.158	-0.359
H(0)		3.970e-35				
	H2	1.985e-35	2.012e-35	-34.702	-34.696	0.006
K		1.053e-02				
	K+	1.019e-02	8.182e-03	-1.992	-2.087	-0.095
	KSO4-	3.248e-04	2.641e-04	-3.488	-3.578	-0.090
	KOH	1.724e-05	1.748e-05	-4.764	-4.758	0.006
	KHPO4-	1.871e-12	1.522e-12	-11.728	-11.818	-0.090
Mg		2.892e-06				
	Mg+2	1.189e-06	5.565e-07	-5.925	-6.255	-0.330
	MgOH+	7.569e-07	6.154e-07	-6.121	-6.211	-0.090
	MgSO4	5.540e-07	5.617e-07	-6.257	-6.251	0.006
	MgCO3	3.843e-07	3.896e-07	-6.415	-6.409	0.006
	MgF+	6.914e-09	5.622e-09	-8.160	-8.250	-0.090
	MgHCO3+	2.630e-10	2.139e-10	-9.580	-9.670	-0.090
	MgPO4-	5.256e-11	4.273e-11	-10.279	-10.369	-0.090
	MgHPO4	3.355e-14	3.401e-14	-13.474	-13.468	0.006
	MgH2PO4+	4.995e-20	4.062e-20	-19.301	-19.391	-0.090
N(5)		1.570e-03				
	NO3-	1.570e-03	1.250e-03	-2.804	-2.903	-0.099
	PbNO3+	1.176e-17	9.563e-18	-16.930	-17.019	-0.090
Na		5.679e-03				
	Na+	5.467e-03	4.456e-03	-2.262	-2.351	-0.089
	NaSO4-	1.376e-04	1.119e-04	-3.861	-3.951	-0.090
	NaCO3-	5.678e-05	4.617e-05	-4.246	-4.336	-0.090
	NaOH	1.789e-05	1.814e-05	-4.747	-4.741	0.006
	NaF	4.454e-07	4.516e-07	-6.351	-6.345	0.006
	NaHCO3	8.345e-08	8.461e-08	-7.079	-7.073	0.006
	NaHPO4-	1.019e-12	8.287e-13	-11.992	-12.082	-0.090
O(0)		6.164e-26				
	O2	3.082e-26	3.125e-26	-25.511	-25.505	0.006
P		3.174e-07				
	CaPO4-	3.167e-07	2.575e-07	-6.499	-6.589	-0.090
	HPO4-2	2.251e-10	9.538e-11	-9.648	-10.021	-0.373
	CaHPO4	2.017e-10	2.045e-10	-9.695	-9.689	0.006
	PO4-3	1.566e-10	2.269e-11	-9.805	-10.644	-0.839
	MgPO4-	5.256e-11	4.273e-11	-10.279	-10.369	-0.090
	KHPO4-	1.871e-12	1.522e-12	-11.728	-11.818	-0.090
	NaHPO4-	1.019e-12	8.287e-13	-11.992	-12.082	-0.090
	MgHPO4	3.355e-14	3.401e-14	-13.474	-13.468	0.006
	H2PO4-	3.206e-15	2.603e-15	-14.494	-14.585	-0.090
	CaH2PO4+	3.189e-16	2.593e-16	-15.496	-15.586	-0.090
	MgH2PO4+	4.995e-20	4.062e-20	-19.301	-19.391	-0.090
Pb		4.848e-08				
	Pb(OH)4-2	3.400e-08	1.486e-08	-7.468	-7.828	-0.359

	Pb(OH) 3-	1.295e-08	1.053e-08	-7.888	-7.977	-0.090
	Pb(OH) 2	1.469e-09	1.489e-09	-8.833	-8.827	0.006
	Pb(CO3) 2-2	3.513e-11	1.535e-11	-10.454	-10.814	-0.359
	PbOH+	7.643e-12	6.214e-12	-11.117	-11.207	-0.090
	PbCO3	7.312e-12	7.413e-12	-11.136	-11.130	0.006
	PbSO4	1.510e-15	1.531e-15	-14.821	-14.815	0.006
	Pb+2	1.184e-15	5.174e-16	-14.927	-15.286	-0.359
	Pb(SO4) 2-2	9.677e-17	4.230e-17	-16.014	-16.374	-0.359
	PbCl+	3.325e-17	2.704e-17	-16.478	-16.568	-0.090
	PbHCO3+	1.707e-17	1.388e-17	-16.768	-16.858	-0.090
	PbNO3+	1.176e-17	9.563e-18	-16.930	-17.019	-0.090
	PbCl2	7.786e-20	7.894e-20	-19.109	-19.103	0.006
	PbCl3-	1.170e-22	9.516e-23	-21.932	-22.022	-0.090
	Pb2OH+3	4.634e-25	7.198e-26	-24.334	-25.143	-0.809
	PbCl4-2	1.563e-25	6.831e-26	-24.806	-25.166	-0.359
S(6)		1.673e-02				
	SO4-2	1.189e-02	5.263e-03	-1.925	-2.279	-0.354
	CaSO4	4.357e-03	4.417e-03	-2.361	-2.355	0.006
	KSO4-	3.248e-04	2.641e-04	-3.488	-3.578	-0.090
	NaSO4-	1.376e-04	1.119e-04	-3.861	-3.951	-0.090
	SrSO4	1.486e-05	1.507e-05	-4.828	-4.822	0.006
	BaSO4	1.127e-06	1.142e-06	-5.948	-5.942	0.006
	MgSO4	5.540e-07	5.617e-07	-6.257	-6.251	0.006
	HSO4-	8.693e-13	7.068e-13	-12.061	-12.151	-0.090
	CaHSO4+	4.728e-14	3.845e-14	-13.325	-13.415	-0.090
	PbSO4	1.510e-15	1.531e-15	-14.821	-14.815	0.006
	Pb(SO4) 2-2	9.677e-17	4.230e-17	-16.014	-16.374	-0.359
	CuSO4	3.842e-17	3.895e-17	-16.415	-16.409	0.006
	AlSO4+	1.287e-27	1.047e-27	-26.890	-26.980	-0.090
	Al(SO4) 2-	2.066e-28	1.680e-28	-27.685	-27.775	-0.090
	AlHSO4+2	3.244e-40	1.418e-40	-39.489	-39.848	-0.359
Si		9.695e-05				
	H3SiO4-	9.163e-05	7.450e-05	-4.038	-4.128	-0.090
	H2SiO4-2	4.259e-06	1.862e-06	-5.371	-5.730	-0.359
	H4SiO4	1.067e-06	1.082e-06	-5.972	-5.966	0.006
	SiF6-2	0.000e+00	0.000e+00	-44.798	-45.158	-0.359
Sr		5.731e-05				
	Sr+2	3.515e-05	1.609e-05	-4.454	-4.793	-0.339
	SrSO4	1.486e-05	1.507e-05	-4.828	-4.822	0.006
	SrCO3	6.675e-06	6.768e-06	-5.176	-5.170	0.006
	SrOH+	6.225e-07	5.084e-07	-6.206	-6.294	-0.088
	SrHCO3+	7.810e-09	6.408e-09	-8.107	-8.193	-0.086

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

Phase	SI	log IAP	log KT	
Al(OH) 3 (a)	-4.10	7.21	11.31	Al(OH) 3
Albite	-6.22	-1.24	4.98	NaAlSi3O8
Alunite	-19.94	-20.38	-0.44	KAl3(SO4)2(OH)6
Anglesite	-9.73	-17.56	-7.83	PbSO4
Anhydrite	-0.28	-4.62	-4.34	CaSO4
Anorthite	-3.29	23.73	27.02	CaAl2Si2O8
Aragonite	2.86	-5.43	-8.29	CaCO3
Barite	1.46	-8.64	-10.10	BaSO4
Ca-Montmorillonite	-10.14	-1.58	8.56	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	3.01	-5.43	-8.44	CaCO3

Celestite	-0.45	-7.07	-6.62	SrSO4
Cerrusite	-5.15	-18.37	-13.22	PbCO3
Chalcedony	-2.32	-5.96	-3.64	SiO2
Chlorite(14A)	11.87	83.15	71.28	Mg5Al2Si3O10(OH)8
Chrysotile	6.88	40.04	33.17	Mg3Si2O5(OH)4
CO2(g)	-8.49	-26.66	-18.18	CO2
Dolomite	2.14	-14.77	-16.91	CaMg(CO3)2
Fluorite	0.84	-9.85	-10.69	CaF2
Gibbsite	-1.34	7.21	8.55	Al(OH)3
Gypsum	-0.04	-4.62	-4.58	CaSO4:2H2O
H2(g)	-31.58	-31.58	0.00	H2
Hydroxyapatite	8.10	-31.87	-39.97	Ca5(PO4)3OH
Illite	-6.82	5.86	12.68	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	-3.29	-0.98	2.31	KAlSi3O8
K-mica	-0.40	13.44	13.84	KAl3Si3O10(OH)2
Kaolinite	-5.62	2.49	8.11	Al2Si2O5(OH)4
O2(g)	-22.58	63.16	85.74	O2
Pb(OH)2	-0.13	8.29	8.42	Pb(OH)2
Quartz	-1.87	-5.96	-4.10	SiO2
Sepiolite	0.79	16.75	15.97	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-1.91	16.75	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-3.19	-5.96	-2.78	SiO2
Strontianite	1.39	-7.88	-9.27	SrCO3
Talc	5.83	28.11	22.29	Mg3Si4O10(OH)2
Witherite	-0.86	-9.45	-8.59	BaCO3

End of simulation.

Reading input data for simulation 2.

End of run.

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

SOLUTION 1 Cell 2B
temp 12.5
pH 13.1
pe 4
redox pe
units mg/l
density 1
Al 1.42
B 0.26
Ba 0.33
Br 8.3
C(4) 450
Ca 1210
Cl 155
Cu 0.02
F 4.7
K 1210
Mg 0.07
N(5) 19.8
Na 220 charge
P 2.11e-07 Mol/l
Pb 0.01
S(6) 2850
Si 5.9
Sr 14.1

Beginning of initial solution calculations.

Initial solution 1. Cell 2B

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

Elements	Molality	Moles
Al	5.295e-05	5.295e-05
B	2.420e-05	2.420e-05
Ba	2.418e-06	2.418e-06
Br	1.045e-04	1.045e-04
C(4)	7.420e-03	7.420e-03
Ca	3.038e-02	3.038e-02

Cl	4.399e-03	4.399e-03	
Cu	3.167e-07	3.167e-07	
F	2.489e-04	2.489e-04	
K	3.114e-02	3.114e-02	
Mg	2.897e-06	2.897e-06	
N(5)	1.422e-03	1.422e-03	
Na	6.623e-02	6.623e-02	Charge balance
P	2.123e-07	2.123e-07	
Pb	4.856e-08	4.856e-08	
S(6)	2.985e-02	2.985e-02	
Si	9.880e-05	9.880e-05	
Sr	1.619e-04	1.619e-04	

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

pH = 13.100
 pe = 4.000
 Activity of water = 0.996
 Ionic strength = 1.571e-01
 Mass of water (kg) = 1.000e+00
 Total alkalinity (eq/kg) = 9.274e-02
 Total CO2 (mol/kg) = 7.420e-03
 Temperature (deg C) = 12.500
 Electrical balance (eq) = 1.766e-13
 Iterations = 9
 Total H = 1.110905e+02
 Total O = 5.573035e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.251e-02	4.568e-02	-1.204	-1.340	-0.136
H+	9.805e-14	7.943e-14	-13.009	-13.100	-0.091
H2O	5.551e+01	9.962e-01	-0.002	-0.002	0.000
Al	5.295e-05				
Al(OH)4-	5.295e-05	4.034e-05	-4.276	-4.394	-0.118
Al(OH)3	1.861e-12	1.930e-12	-11.730	-11.714	0.016
Al(OH)2+	3.736e-18	2.846e-18	-17.428	-17.546	-0.118
AlOH2+	2.790e-25	9.393e-26	-24.554	-25.027	-0.473
AlF3	4.797e-28	4.973e-28	-27.319	-27.303	0.016
AlF2+	3.011e-28	2.294e-28	-27.521	-27.639	-0.118
AlF4-	4.524e-29	3.446e-29	-28.344	-28.463	-0.118
AlF+2	8.335e-30	2.806e-30	-29.079	-29.552	-0.473
AlF5-2	2.908e-31	9.790e-32	-30.536	-31.009	-0.473
AlSO4+	4.375e-32	3.332e-32	-31.359	-31.477	-0.118
Al+3	1.157e-32	1.738e-33	-31.937	-32.760	-0.823
Al(SO4)2-	9.347e-33	7.119e-33	-32.029	-32.148	-0.118
AlF6-3	2.565e-34	2.215e-35	-33.591	-34.655	-1.064
AlHSO4+2	0.000e+00	0.000e+00	-45.195	-45.668	-0.473
B	2.420e-05				
H2BO3-	2.420e-05	1.843e-05	-4.616	-4.734	-0.118
H3BO3	3.114e-09	3.228e-09	-8.507	-8.491	0.016
BF(OH)3-	2.569e-13	1.957e-13	-12.590	-12.708	-0.118
BF2(OH)2-	3.897e-22	2.969e-22	-21.409	-21.527	-0.118
BF3OH-	7.551e-33	5.752e-33	-32.122	-32.240	-0.118

	BF4-	0.000e+00	0.000e+00	-42.361	-42.479	-0.118
Ba		2.418e-06				
	BaSO4	1.136e-06	1.178e-06	-5.945	-5.929	0.016
	Ba+2	9.903e-07	3.274e-07	-6.004	-6.485	-0.481
	BaOH+	1.826e-07	1.391e-07	-6.738	-6.857	-0.118
	BaCO3	1.089e-07	1.129e-07	-6.963	-6.947	0.016
	BaHCO3+	5.430e-12	4.136e-12	-11.265	-11.383	-0.118
Br		1.045e-04				
	Br-	1.045e-04	7.527e-05	-3.981	-4.123	-0.143
C(4)		7.420e-03				
	CaCO3	4.400e-03	4.562e-03	-2.357	-2.341	0.016
	CO3-2	2.509e-03	8.580e-04	-2.600	-3.067	-0.466
	NaCO3-	4.966e-04	3.783e-04	-3.304	-3.422	-0.118
	SrCO3	1.136e-05	1.178e-05	-4.944	-4.929	0.016
	HCO3-	2.555e-06	1.953e-06	-5.593	-5.709	-0.117
	BaCO3	1.089e-07	1.129e-07	-6.963	-6.947	0.016
	CaHCO3+	9.685e-08	7.406e-08	-7.014	-7.130	-0.117
	MgCO3	8.236e-08	8.539e-08	-7.084	-7.069	0.016
	NaHCO3	4.844e-08	5.023e-08	-7.315	-7.299	0.016
	SrHCO3+	7.927e-10	6.061e-10	-9.101	-9.217	-0.117
	BaHCO3+	5.430e-12	4.136e-12	-11.265	-11.383	-0.118
	MgHCO3+	3.648e-12	2.779e-12	-11.438	-11.556	-0.118
	CO2	4.138e-13	4.290e-13	-12.383	-12.368	0.016
	Pb(CO3)2-2	3.113e-16	1.048e-16	-15.507	-15.980	-0.473
	PbCO3	4.690e-17	4.863e-17	-16.329	-16.313	0.016
	PbHCO3+	6.643e-24	5.060e-24	-23.178	-23.296	-0.118
Ca		3.038e-02				
	Ca+2	1.088e-02	3.816e-03	-1.964	-2.418	-0.455
	CaOH+	1.043e-02	7.943e-03	-1.982	-2.100	-0.118
	CaSO4	4.667e-03	4.839e-03	-2.331	-2.315	0.016
	CaCO3	4.400e-03	4.562e-03	-2.357	-2.341	0.016
	CaF+	5.619e-06	4.280e-06	-5.250	-5.369	-0.118
	CaPO4-	2.120e-07	1.615e-07	-6.674	-6.792	-0.118
	CaHCO3+	9.685e-08	7.406e-08	-7.014	-7.130	-0.117
	CaHPO4	6.687e-12	6.933e-12	-11.175	-11.159	0.016
	CaHSO4+	2.580e-15	1.965e-15	-14.588	-14.707	-0.118
	CaH2PO4+	5.804e-19	4.421e-19	-18.236	-18.355	-0.118
Cl		4.399e-03				
	Cl-	4.399e-03	3.232e-03	-2.357	-2.491	-0.134
	PbCl+	3.986e-22	3.036e-22	-21.399	-21.518	-0.118
	PbCl2	1.914e-24	1.985e-24	-23.718	-23.702	0.016
	PbCl3-	6.172e-27	4.701e-27	-26.210	-26.328	-0.118
	PbCl4-2	1.954e-29	6.577e-30	-28.709	-29.182	-0.473
Cu(1)		8.340e-22				
	Cu+	8.340e-22	5.911e-22	-21.079	-21.228	-0.150
Cu(2)		3.167e-07				
	Cu(OH)4-2	2.349e-07	7.907e-08	-6.629	-7.102	-0.473
	Cu(OH)3-	4.148e-08	3.160e-08	-7.382	-7.500	-0.118
	Cu(OH)2	4.032e-08	4.181e-08	-7.394	-7.379	0.016
	CuOH+	2.155e-15	1.596e-15	-14.667	-14.797	-0.130
	Cu+2	3.550e-20	1.272e-20	-19.450	-19.895	-0.446
	CuSO4	1.643e-20	1.704e-20	-19.784	-19.769	0.016
F		2.489e-04				
	F-	2.389e-04	1.746e-04	-3.622	-3.758	-0.136
	CaF+	5.619e-06	4.280e-06	-5.250	-5.369	-0.118
	NaF	4.429e-06	4.593e-06	-5.354	-5.338	0.016
	MgF+	1.511e-09	1.151e-09	-8.821	-8.939	-0.118

	BF(OH) 3-	2.569e-13	1.957e-13	-12.590	-12.708	-0.118
	HF	1.611e-14	1.670e-14	-13.793	-13.777	0.016
	HF2-	1.307e-17	9.952e-18	-16.884	-17.002	-0.118
	BF2(OH) 2-	3.897e-22	2.969e-22	-21.409	-21.527	-0.118
	AlF3	4.797e-28	4.973e-28	-27.319	-27.303	0.016
	AlF2+	3.011e-28	2.294e-28	-27.521	-27.639	-0.118
	AlF4-	4.524e-29	3.446e-29	-28.344	-28.463	-0.118
	AlF+2	8.335e-30	2.806e-30	-29.079	-29.552	-0.473
	AlF5-2	2.908e-31	9.790e-32	-30.536	-31.009	-0.473
	BF3OH-	7.551e-33	5.752e-33	-32.122	-32.240	-0.118
	AlF6-3	2.565e-34	2.215e-35	-33.591	-34.655	-1.064
	BF4-	0.000e+00	0.000e+00	-42.361	-42.479	-0.118
	SiF6-2	0.000e+00	0.000e+00	-51.211	-51.684	-0.473
H(0)		9.812e-38				
	H2	4.906e-38	5.087e-38	-37.309	-37.294	0.016
K		3.114e-02				
	K+	2.911e-02	2.139e-02	-1.536	-1.670	-0.134
	KSO4-	1.128e-03	8.591e-04	-2.948	-3.066	-0.118
	KOH	8.971e-04	9.301e-04	-3.047	-3.031	0.016
	KHPO4-	2.315e-13	1.763e-13	-12.635	-12.754	-0.118
Mg		2.897e-06				
	MgOH+	2.326e-06	1.771e-06	-5.633	-5.752	-0.118
	Mg+2	3.410e-07	1.264e-07	-6.467	-6.898	-0.431
	MgSO4	1.466e-07	1.520e-07	-6.834	-6.818	0.016
	MgCO3	8.236e-08	8.539e-08	-7.084	-7.069	0.016
	MgF+	1.511e-09	1.151e-09	-8.821	-8.939	-0.118
	MgPO4-	9.469e-12	7.213e-12	-11.024	-11.142	-0.118
	MgHCO3+	3.648e-12	2.779e-12	-11.438	-11.556	-0.118
	MgHPO4	2.994e-16	3.104e-16	-15.524	-15.508	0.016
	MgH2PO4+	2.447e-23	1.864e-23	-22.611	-22.730	-0.118
N(5)		1.422e-03				
	NO3-	1.422e-03	1.024e-03	-2.847	-2.990	-0.143
	PbNO3+	6.486e-23	4.941e-23	-22.188	-22.306	-0.118
Na		6.623e-02				
	Na+	6.009e-02	4.572e-02	-1.221	-1.340	-0.119
	NaOH	3.654e-03	3.789e-03	-2.437	-2.422	0.016
	NaSO4-	1.988e-03	1.514e-03	-2.702	-2.820	-0.118
	NaCO3-	4.966e-04	3.783e-04	-3.304	-3.422	-0.118
	NaF	4.429e-06	4.593e-06	-5.354	-5.338	0.016
	NaHCO3	4.844e-08	5.023e-08	-7.315	-7.299	0.016
	NaHPO4-	4.949e-13	3.769e-13	-12.306	-12.424	-0.118
O(0)		1.899e-22				
	O2	9.497e-23	9.847e-23	-22.022	-22.007	0.016
P		2.123e-07				
	CaPO4-	2.120e-07	1.615e-07	-6.674	-6.792	-0.118
	PO4-3	2.759e-10	1.849e-11	-9.559	-10.733	-1.174
	HPO4-2	1.406e-11	4.228e-12	-10.852	-11.374	-0.522
	MgPO4-	9.469e-12	7.213e-12	-11.024	-11.142	-0.118
	CaHPO4	6.687e-12	6.933e-12	-11.175	-11.159	0.016
	NaHPO4-	4.949e-13	3.769e-13	-12.306	-12.424	-0.118
	KHPO4-	2.315e-13	1.763e-13	-12.635	-12.754	-0.118
	MgHPO4	2.994e-16	3.104e-16	-15.524	-15.508	0.016
	H2PO4-	7.762e-18	5.820e-18	-17.110	-17.235	-0.125
	CaH2PO4+	5.804e-19	4.421e-19	-18.236	-18.355	-0.118
	MgH2PO4+	2.447e-23	1.864e-23	-22.611	-22.730	-0.118
Pb		4.856e-08				
	Pb(OH) 4-2	4.782e-08	1.610e-08	-7.320	-7.793	-0.473

	Pb(OH) 3-	7.356e-10	5.603e-10	-9.133	-9.252	-0.118
	Pb(OH) 2	3.753e-12	3.891e-12	-11.426	-11.410	0.016
	PbOH+	1.047e-15	7.975e-16	-14.980	-15.098	-0.118
	Pb(CO3) 2-2	3.113e-16	1.048e-16	-15.507	-15.980	-0.473
	PbCO3	4.690e-17	4.863e-17	-16.329	-16.313	0.016
	PbSO4	1.270e-20	1.316e-20	-19.896	-19.881	0.016
	Pb+2	9.687e-21	3.261e-21	-20.014	-20.487	-0.473
	Pb(SO4) 2-2	1.473e-21	4.959e-22	-20.832	-21.305	-0.473
	PbCl+	3.986e-22	3.036e-22	-21.399	-21.518	-0.118
	PbNO3+	6.486e-23	4.941e-23	-22.188	-22.306	-0.118
	PbHCO3+	6.643e-24	5.060e-24	-23.178	-23.296	-0.118
	PbCl2	1.914e-24	1.985e-24	-23.718	-23.702	0.016
	PbCl3-	6.172e-27	4.701e-27	-26.210	-26.328	-0.118
	PbCl4-2	1.954e-29	6.577e-30	-28.709	-29.182	-0.473
	Pb2OH+3	6.745e-34	5.822e-35	-33.171	-34.235	-1.064
S(6)		2.985e-02				
	SO4-2	2.203e-02	7.178e-03	-1.657	-2.144	-0.487
	CaSO4	4.667e-03	4.839e-03	-2.331	-2.315	0.016
	NaSO4-	1.988e-03	1.514e-03	-2.702	-2.820	-0.118
	KSO4-	1.128e-03	8.591e-04	-2.948	-3.066	-0.118
	SrSO4	3.603e-05	3.735e-05	-4.443	-4.428	0.016
	BaSO4	1.136e-06	1.178e-06	-5.945	-5.929	0.016
	MgSO4	1.466e-07	1.520e-07	-6.834	-6.818	0.016
	HSO4-	5.623e-14	4.283e-14	-13.250	-13.368	-0.118
	CaHSO4+	2.580e-15	1.965e-15	-14.588	-14.707	-0.118
	CuSO4	1.643e-20	1.704e-20	-19.784	-19.769	0.016
	PbSO4	1.270e-20	1.316e-20	-19.896	-19.881	0.016
	Pb(SO4) 2-2	1.473e-21	4.959e-22	-20.832	-21.305	-0.473
	AlSO4+	4.375e-32	3.332e-32	-31.359	-31.477	-0.118
	Al(SO4) 2-	9.347e-33	7.119e-33	-32.029	-32.148	-0.118
	AlHSO4+2	0.000e+00	0.000e+00	-45.195	-45.668	-0.473
Si		9.880e-05				
	H3SiO4-	5.469e-05	4.166e-05	-4.262	-4.380	-0.118
	H2SiO4-2	4.408e-05	1.484e-05	-4.356	-4.829	-0.473
	H4SiO4	3.472e-08	3.600e-08	-7.459	-7.444	0.016
	SiF6-2	0.000e+00	0.000e+00	-51.211	-51.684	-0.473
Sr		1.619e-04				
	Sr+2	8.813e-05	3.112e-05	-4.055	-4.507	-0.452
	SrSO4	3.603e-05	3.735e-05	-4.443	-4.428	0.016
	SrOH+	2.640e-05	2.002e-05	-4.578	-4.699	-0.120
	SrCO3	1.136e-05	1.178e-05	-4.944	-4.929	0.016
	SrHCO3+	7.927e-10	6.061e-10	-9.101	-9.217	-0.117

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

Phase	SI	log IAP	log KT	
Al(OH) 3 (a)	-5.11	6.54	11.65	Al(OH) 3
Albite	-9.22	-4.02	5.20	NaAlSi3O8
Alunite	-25.86	-25.65	0.21	KAl3(SO4)2(OH)6
Anglesite	-14.77	-22.63	-7.86	PbSO4
Anhydrite	-0.23	-4.56	-4.33	CaSO4
Anorthite	-6.00	21.97	27.97	CaAl2Si2O8
Aragonite	2.78	-5.48	-8.27	CaCO3
Barite	1.56	-8.63	-10.19	BaSO4
Ca-Montmorillonite	-17.24	-8.15	9.09	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	2.94	-5.48	-8.42	CaCO3

Celestite	-0.03	-6.65	-6.62	SrSO4
Cerrusite	-10.27	-23.55	-13.29	PbCO3
Chalcedony	-3.74	-7.44	-3.70	SiO2
Chlorite(14A)	14.01	87.25	73.24	Mg5Al2Si3O10(OH)8
Chrysotile	9.20	43.02	33.82	Mg3Si2O5(OH)4
CO2(g)	-11.06	-29.26	-18.20	CO2
Dolomite	1.34	-15.45	-16.79	CaMg(CO3)2
Fluorite	0.83	-9.93	-10.76	CaF2
Gibbsite	-2.31	6.54	8.84	Al(OH)3
Gypsum	0.02	-4.57	-4.59	CaSO4:2H2O
H2(g)	-34.20	-34.20	0.00	H2
Hydroxyapatite	8.45	-31.19	-39.64	Ca5(PO4)3OH
Illite	-12.57	0.68	13.24	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	-6.82	-4.35	2.47	KAlSi3O8
K-mica	-5.89	8.72	14.61	KAl3Si3O10(OH)2
Kaolinite	-10.38	-1.81	8.57	Al2Si2O5(OH)4
O2(g)	-19.11	68.40	87.50	O2
Pb(OH)2	-2.89	5.71	8.60	Pb(OH)2
Quartz	-3.27	-7.44	-4.17	SiO2
Sepiolite	0.17	16.27	16.10	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-2.39	16.27	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-4.62	-7.44	-2.82	SiO2
Strontianite	1.71	-7.57	-9.28	SrCO3
Talc	5.25	28.14	22.89	Mg3Si4O10(OH)2
Witherite	-0.94	-9.55	-8.61	BaCO3

End of simulation.

Reading input data for simulation 2.

End of run.

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

SOLUTION 1 Cell 3B
temp 17
pH 12.52
pe 4
redox pe
units mg/l
density 1
Al 0.97
B 0.26
Ba 0.26
Br 2.6
C(4) 450
Ca 760
Cl 60
F 3.1
K 350
Mg 0.1
N(5) 22.3
Na 125 charge
P 2.11e-07 Mol/l
Pb 0.01
S(6) 1400
Si 8.2
Sr 5.1

Beginning of initial solution calculations.

Initial solution 1. Cell 3B

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

Elements	Molality	Moles
Al	3.607e-05	3.607e-05
B	2.413e-05	2.413e-05
Ba	1.899e-06	1.899e-06
Br	3.264e-05	3.264e-05
C(4)	7.398e-03	7.398e-03
Ca	1.902e-02	1.902e-02
Cl	1.698e-03	1.698e-03

F	1.637e-04	1.637e-04	
K	8.980e-03	8.980e-03	
Mg	4.126e-06	4.126e-06	
N(5)	1.597e-03	1.597e-03	
Na	2.603e-02	2.603e-02	Charge balance
P	2.117e-07	2.117e-07	
Pb	4.842e-08	4.842e-08	
S(6)	1.462e-02	1.462e-02	
Si	1.369e-04	1.369e-04	
Sr	5.839e-05	5.839e-05	

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

pH	=	12.520
pe	=	4.000
Activity of water	=	0.998
Ionic strength	=	7.489e-02
Mass of water (kg)	=	1.000e+00
Total alkalinity (eq/kg)	=	4.056e-02
Total CO2 (mol/kg)	=	7.398e-03
Temperature (deg C)	=	17.000
Electrical balance (eq)	=	-1.340e-15
Iterations	=	11
Total H	=	1.110385e+02
Total O	=	5.561788e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.240e-02	1.760e-02	-1.650	-1.754	-0.105
H+	3.599e-13	3.020e-13	-12.444	-12.520	-0.076
H2O	5.551e+01	9.984e-01	-0.001	-0.001	0.000
Al	3.607e-05				
Al(OH)4-	3.607e-05	2.887e-05	-4.443	-4.540	-0.097
Al(OH)3	4.982e-12	5.069e-12	-11.303	-11.295	0.007
Al(OH)2+	2.421e-17	1.938e-17	-16.616	-16.713	-0.097
AlOH+2	3.792e-24	1.556e-24	-23.421	-23.808	-0.387
AlF3	8.663e-27	8.813e-27	-26.062	-26.055	0.007
AlF2+	7.097e-27	5.680e-27	-26.149	-26.246	-0.097
AlF4-	5.438e-28	4.352e-28	-27.265	-27.361	-0.097
AlF+2	2.320e-28	9.518e-29	-27.635	-28.021	-0.387
AlF5-2	2.125e-30	8.718e-31	-29.673	-30.060	-0.387
AlSO4+	1.283e-30	1.026e-30	-29.892	-29.989	-0.097
Al+3	3.902e-31	8.045e-32	-30.409	-31.094	-0.686
Al(SO4)2-	1.752e-31	1.402e-31	-30.756	-30.853	-0.097
AlF6-3	9.468e-34	1.276e-34	-33.024	-33.894	-0.870
AlHSO4+2	0.000e+00	0.000e+00	-43.201	-43.588	-0.387
B	2.413e-05				
H2BO3-	2.412e-05	1.930e-05	-4.618	-4.714	-0.097
H3BO3	1.157e-08	1.177e-08	-7.937	-7.929	0.007
BF(OH)3-	6.676e-13	5.343e-13	-12.175	-12.272	-0.097
BF2(OH)2-	2.718e-21	2.176e-21	-20.566	-20.662	-0.097
BF3OH-	1.302e-31	1.042e-31	-30.885	-30.982	-0.097
BF4-	0.000e+00	0.000e+00	-40.695	-40.792	-0.097
Ba	1.899e-06				

	Ba+2	8.846e-07	3.686e-07	-6.053	-6.433	-0.380
	BaSO4	8.151e-07	8.292e-07	-6.089	-6.081	0.007
	BaCO3	1.479e-07	1.504e-07	-6.830	-6.823	0.007
	BaOH+	5.160e-08	4.130e-08	-7.287	-7.384	-0.097
	BaHCO3+	2.452e-11	1.962e-11	-10.611	-10.707	-0.097
Br		3.264e-05				
	Br-	3.264e-05	2.543e-05	-4.486	-4.595	-0.108
C(4)		7.398e-03				
	CaCO3	4.919e-03	5.004e-03	-2.308	-2.301	0.007
	CO3-2	2.179e-03	9.276e-04	-2.662	-3.033	-0.371
	NaCO3-	2.835e-04	2.269e-04	-3.548	-3.644	-0.097
	HCO3-	8.844e-06	7.143e-06	-5.053	-5.146	-0.093
	SrCO3	7.119e-06	7.243e-06	-5.148	-5.140	0.007
	CaHCO3+	3.590e-07	2.900e-07	-6.445	-6.538	-0.093
	MgCO3	2.883e-07	2.933e-07	-6.540	-6.533	0.007
	BaCO3	1.479e-07	1.504e-07	-6.830	-6.823	0.007
	NaHCO3	7.850e-08	7.986e-08	-7.105	-7.098	0.007
	SrHCO3+	1.594e-09	1.287e-09	-8.798	-8.890	-0.093
	MgHCO3+	3.802e-11	3.043e-11	-10.420	-10.517	-0.097
	BaHCO3+	2.452e-11	1.962e-11	-10.611	-10.707	-0.097
	CO2	5.373e-12	5.467e-12	-11.270	-11.262	0.007
	Pb(CO3)2-2	7.137e-14	2.928e-14	-13.147	-13.533	-0.387
	PbCO3	1.235e-14	1.257e-14	-13.908	-13.901	0.007
	PbHCO3+	5.527e-21	4.423e-21	-20.258	-20.354	-0.097
Ca		1.902e-02				
	Ca+2	8.579e-03	3.678e-03	-2.067	-2.434	-0.368
	CaCO3	4.919e-03	5.004e-03	-2.308	-2.301	0.007
	CaSO4	2.998e-03	3.051e-03	-2.523	-2.516	0.007
	CaOH+	2.522e-03	2.018e-03	-2.598	-2.695	-0.097
	CaF+	4.107e-06	3.287e-06	-5.386	-5.483	-0.097
	CaHCO3+	3.590e-07	2.900e-07	-6.445	-6.538	-0.093
	CaPO4-	2.114e-07	1.692e-07	-6.675	-6.772	-0.097
	CaHPO4	2.479e-11	2.522e-11	-10.606	-10.598	0.007
	CaHSO4+	6.151e-15	4.923e-15	-14.211	-14.308	-0.097
	CaH2PO4+	7.455e-18	5.967e-18	-17.128	-17.224	-0.097
Cl		1.698e-03				
	Cl-	1.698e-03	1.337e-03	-2.770	-2.874	-0.104
	PbCl+	4.230e-20	3.385e-20	-19.374	-19.470	-0.097
	PbCl2	8.224e-23	8.367e-23	-22.085	-22.077	0.007
	PbCl3-	1.056e-25	8.449e-26	-24.976	-25.073	-0.097
	PbCl4-2	1.237e-28	5.076e-29	-27.908	-28.294	-0.387
F		1.637e-04				
	F-	1.582e-04	1.243e-04	-3.801	-3.906	-0.105
	CaF+	4.107e-06	3.287e-06	-5.386	-5.483	-0.097
	NaF	1.398e-06	1.422e-06	-5.855	-5.847	0.007
	MgF+	3.312e-09	2.651e-09	-8.480	-8.577	-0.097
	BF(OH)3-	6.676e-13	5.343e-13	-12.175	-12.272	-0.097
	HF	4.802e-14	4.886e-14	-13.319	-13.311	0.007
	HF2-	2.714e-17	2.172e-17	-16.566	-16.663	-0.097
	BF2(OH)2-	2.718e-21	2.176e-21	-20.566	-20.662	-0.097
	AlF3	8.663e-27	8.813e-27	-26.062	-26.055	0.007
	AlF2+	7.097e-27	5.680e-27	-26.149	-26.246	-0.097
	AlF4-	5.438e-28	4.352e-28	-27.265	-27.361	-0.097
	AlF+2	2.320e-28	9.518e-29	-27.635	-28.021	-0.387
	AlF5-2	2.125e-30	8.718e-31	-29.673	-30.060	-0.387
	BF3OH-	1.302e-31	1.042e-31	-30.885	-30.982	-0.097
	AlF6-3	9.468e-34	1.276e-34	-33.024	-33.894	-0.870

	BF4-	0.000e+00	0.000e+00	-40.695	-40.792	-0.097
	SiF6-2	0.000e+00	0.000e+00	-49.236	-49.623	-0.387
H (0)		1.377e-36				
	H2	6.887e-37	7.007e-37	-36.162	-36.154	0.007
K		8.980e-03				
	K+	8.669e-03	6.829e-03	-2.062	-2.166	-0.104
	KSO4-	2.331e-04	1.866e-04	-3.632	-3.729	-0.097
	KOH	7.695e-05	7.828e-05	-4.114	-4.106	0.007
	KHPO4-	2.426e-13	1.942e-13	-12.615	-12.712	-0.097
Mg		4.126e-06				
	MgOH+	2.675e-06	2.141e-06	-5.573	-5.669	-0.097
	Mg+2	8.462e-07	3.747e-07	-6.073	-6.426	-0.354
	MgSO4	3.136e-07	3.190e-07	-6.504	-6.496	0.007
	MgCO3	2.883e-07	2.933e-07	-6.540	-6.533	0.007
	MgF+	3.312e-09	2.651e-09	-8.480	-8.577	-0.097
	MgHCO3+	3.802e-11	3.043e-11	-10.420	-10.517	-0.097
	MgPO4-	2.905e-11	2.325e-11	-10.537	-10.634	-0.097
	MgHPO4	3.414e-15	3.474e-15	-14.467	-14.459	0.007
	MgH2PO4+	9.671e-22	7.740e-22	-21.015	-21.111	-0.097
N (5)		1.597e-03				
	NO3-	1.597e-03	1.244e-03	-2.797	-2.905	-0.108
	PbNO3+	1.793e-20	1.435e-20	-19.746	-19.843	-0.097
Na		2.603e-02				
	Na+	2.478e-02	1.988e-02	-1.606	-1.702	-0.096
	NaSO4-	5.304e-04	4.245e-04	-3.275	-3.372	-0.097
	NaOH	4.269e-04	4.343e-04	-3.370	-3.362	0.007
	NaCO3-	2.835e-04	2.269e-04	-3.548	-3.644	-0.097
	NaF	1.398e-06	1.422e-06	-5.855	-5.847	0.007
	NaHCO3	7.850e-08	7.986e-08	-7.105	-7.098	0.007
	NaHPO4-	7.063e-13	5.653e-13	-12.151	-12.248	-0.097
O (0)		3.699e-23				
	O2	1.850e-23	1.882e-23	-22.733	-22.725	0.007
P		2.117e-07				
	CaPO4-	2.114e-07	1.692e-07	-6.675	-6.772	-0.097
	PO4-3	1.507e-10	1.847e-11	-9.822	-10.734	-0.912
	HPO4-2	3.707e-11	1.458e-11	-10.431	-10.836	-0.405
	MgPO4-	2.905e-11	2.325e-11	-10.537	-10.634	-0.097
	CaHPO4	2.479e-11	2.522e-11	-10.606	-10.598	0.007
	NaHPO4-	7.063e-13	5.653e-13	-12.151	-12.248	-0.097
	KHPO4-	2.426e-13	1.942e-13	-12.615	-12.712	-0.097
	MgHPO4	3.414e-15	3.474e-15	-14.467	-14.459	0.007
	H2PO4-	9.308e-17	7.427e-17	-16.031	-16.129	-0.098
	CaH2PO4+	7.455e-18	5.967e-18	-17.128	-17.224	-0.097
	MgH2PO4+	9.671e-22	7.740e-22	-21.015	-21.111	-0.097
Pb		4.842e-08				
	Pb (OH) 4-2	4.529e-08	1.858e-08	-7.344	-7.731	-0.387
	Pb (OH) 3-	3.066e-09	2.454e-09	-8.513	-8.610	-0.097
	Pb (OH) 2	6.354e-11	6.464e-11	-10.197	-10.189	0.007
	Pb (CO3) 2-2	7.137e-14	2.928e-14	-13.147	-13.533	-0.387
	PbOH+	6.279e-14	5.026e-14	-13.202	-13.299	-0.097
	PbCO3	1.235e-14	1.257e-14	-13.908	-13.901	0.007
	PbSO4	1.934e-18	1.968e-18	-17.714	-17.706	0.007
	Pb+2	1.900e-18	7.796e-19	-17.721	-18.108	-0.387
	Pb (SO4) 2-2	1.130e-19	4.635e-20	-18.947	-19.334	-0.387
	PbCl+	4.230e-20	3.385e-20	-19.374	-19.470	-0.097
	PbNO3+	1.793e-20	1.435e-20	-19.746	-19.843	-0.097
	PbHCO3+	5.527e-21	4.423e-21	-20.258	-20.354	-0.097

	PbCl2	8.224e-23	8.367e-23	-22.085	-22.077	0.007
	PbCl3-	1.056e-25	8.449e-26	-24.976	-25.073	-0.097
	PbCl4-2	1.237e-28	5.076e-29	-27.908	-28.294	-0.387
	Pb2OH+3	6.509e-30	8.772e-31	-29.186	-30.057	-0.870
S(6)		1.462e-02				
	SO4-2	1.084e-02	4.488e-03	-1.965	-2.348	-0.383
	CaSO4	2.998e-03	3.051e-03	-2.523	-2.516	0.007
	NaSO4-	5.304e-04	4.245e-04	-3.275	-3.372	-0.097
	KSO4-	2.331e-04	1.866e-04	-3.632	-3.729	-0.097
	SrSO4	1.210e-05	1.231e-05	-4.917	-4.910	0.007
	BaSO4	8.151e-07	8.292e-07	-6.089	-6.081	0.007
	MgSO4	3.136e-07	3.190e-07	-6.504	-6.496	0.007
	H2SO4	1.391e-13	1.113e-13	-12.857	-12.953	-0.097
	CaHSO4+	6.151e-15	4.923e-15	-14.211	-14.308	-0.097
	PbSO4	1.934e-18	1.968e-18	-17.714	-17.706	0.007
	Pb(SO4)2-2	1.130e-19	4.635e-20	-18.947	-19.334	-0.387
	AlSO4+	1.283e-30	1.026e-30	-29.892	-29.989	-0.097
	Al(SO4)2-	1.752e-31	1.402e-31	-30.756	-30.853	-0.097
	AlHSO4+2	0.000e+00	0.000e+00	-43.201	-43.588	-0.387
Si		1.369e-04				
	H3SiO4-	1.090e-04	8.720e-05	-3.963	-4.059	-0.097
	H2SiO4-2	2.772e-05	1.137e-05	-4.557	-4.944	-0.387
	H4SiO4	2.354e-07	2.395e-07	-6.628	-6.621	0.007
	SiF6-2	0.000e+00	0.000e+00	-49.236	-49.623	-0.387
Sr		5.839e-05				
	Sr+2	3.591e-05	1.549e-05	-4.445	-4.810	-0.365
	SrSO4	1.210e-05	1.231e-05	-4.917	-4.910	0.007
	SrCO3	7.119e-06	7.243e-06	-5.148	-5.140	0.007
	SrOH+	3.269e-06	2.627e-06	-5.486	-5.581	-0.095
	SrHCO3+	1.594e-09	1.287e-09	-8.798	-8.890	-0.093

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

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-4.87	6.46	11.34	Al(OH)3
Albite	-7.57	-2.58	5.00	NaAlSi3O8
Alunite	-24.64	-25.03	-0.38	KAl3(SO4)2(OH)6
Anglesite	-12.62	-20.46	-7.83	PbSO4
Anhydrite	-0.44	-4.78	-4.34	CaSO4
Anorthite	-4.80	22.30	27.10	CaAl2Si2O8
Aragonite	2.82	-5.47	-8.29	CaCO3
Barite	1.33	-8.78	-10.11	BaSO4
Ca-Montmorillonite	-14.10	-5.50	8.60	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	2.97	-5.47	-8.44	CaCO3
Celestite	-0.54	-7.16	-6.62	SrSO4
Cerrusite	-7.91	-21.14	-13.23	PbCO3
Chalcedony	-2.97	-6.62	-3.65	SiO2
Chlorite(14A)	14.69	86.13	71.44	Mg5Al2Si3O10(OH)8
Chrysotile	9.38	42.60	33.22	Mg3Si2O5(OH)4
CO2(g)	-9.89	-28.07	-18.18	CO2
Dolomite	1.97	-14.93	-16.90	CaMg(CO3)2
Fluorite	0.45	-10.25	-10.70	CaF2
Gibbsite	-2.11	6.46	8.57	Al(OH)3
Gypsum	-0.20	-4.78	-4.58	CaSO4·2H2O
H2(g)	-33.04	-33.04	0.00	H2
Hydroxyapatite	8.09	-31.85	-39.94	Ca5(PO4)3OH

Illite	-10.16	2.57	12.73	K _{0.6} Mg _{0.25} Al _{2.3} Si _{3.5} O ₁₀ (OH) ₂
K-feldspar	-5.37	-3.04	2.33	KAlSi ₃ O ₈
K-mica	-4.01	9.89	13.90	KAl ₃ Si ₃ O ₁₀ (OH) ₂
Kaolinite	-8.46	-0.31	8.15	Al ₂ Si ₂ O ₅ (OH) ₄
O ₂ (g)	-19.80	66.08	85.88	O ₂
Pb(OH) ₂	-1.50	6.93	8.43	Pb(OH) ₂
Quartz	-2.52	-6.62	-4.10	SiO ₂
Sepiolite	1.39	17.37	15.98	Mg ₂ Si ₃ O ₇ .5OH:3H ₂ O
Sepiolite(d)	-1.29	17.37	18.66	Mg ₂ Si ₃ O ₇ .5OH:3H ₂ O
SiO ₂ (a)	-3.84	-6.62	-2.78	SiO ₂
Strontianite	1.43	-7.84	-9.27	SrCO ₃
Talc	7.03	29.36	22.34	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Witherite	-0.88	-9.47	-8.59	BaCO ₃

 End of simulation.

 Reading input data for simulation 2.

 End of run.

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

SOLUTION 1 Cell 4B
temp 19
pH 12.44
pe 4
redox pe
units mg/l
density 1
Al 0.74
B 0.23
Ba 0.32
Br 2.9
C(4) 450
Ca 800
Cl 62
F 3.8
K 350
Mg 0.08
N(5) 21.5
Na 115 charge
P 2.11e-07 Mol/l
Pb 0.01
S(6) 1470
Si 5
Sr 5.5

Beginning of initial solution calculations.

Initial solution 1. Cell 4B

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

Elements	Molality	Moles
Al	2.752e-05	2.752e-05
B	2.135e-05	2.135e-05
Ba	2.338e-06	2.338e-06
Br	3.641e-05	3.641e-05
C(4)	7.399e-03	7.399e-03
Ca	2.003e-02	2.003e-02
Cl	1.755e-03	1.755e-03

F	2.007e-04	2.007e-04	
K	8.980e-03	8.980e-03	
Mg	3.301e-06	3.301e-06	
N(5)	1.540e-03	1.540e-03	
Na	2.465e-02	2.465e-02	Charge balance
P	2.117e-07	2.117e-07	
Pb	4.842e-08	4.842e-08	
S(6)	1.535e-02	1.535e-02	
Si	8.349e-05	8.349e-05	
Sr	6.298e-05	6.298e-05	

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

pH	=	12.440
pe	=	4.000
Activity of water	=	0.998
Ionic strength	=	7.573e-02
Mass of water (kg)	=	1.000e+00
Total alkalinity (eq/kg)	=	3.966e-02
Total CO2 (mol/kg)	=	7.399e-03
Temperature (deg C)	=	19.000
Electrical balance (eq)	=	-1.732e-12
Iterations	=	10
Total H	=	1.110375e+02
Total O	=	5.561959e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.197e-02	1.723e-02	-1.658	-1.764	-0.106
H+	4.331e-13	3.631e-13	-12.363	-12.440	-0.077
H2O	5.551e+01	9.984e-01	-0.001	-0.001	0.000
Al	2.752e-05				
Al(OH)4-	2.752e-05	2.199e-05	-4.560	-4.658	-0.097
Al(OH)3	4.477e-12	4.556e-12	-11.349	-11.341	0.008
Al(OH)2+	2.229e-17	1.781e-17	-16.652	-16.749	-0.097
AlOH+2	3.487e-24	1.422e-24	-23.458	-23.847	-0.389
AlF3	1.552e-26	1.579e-26	-25.809	-25.802	0.008
AlF2+	1.041e-26	8.321e-27	-25.982	-26.080	-0.097
AlF4-	1.191e-27	9.520e-28	-26.924	-27.021	-0.097
AlF+2	2.771e-28	1.130e-28	-27.557	-27.947	-0.389
AlF5-2	5.681e-30	2.317e-30	-29.246	-29.635	-0.389
AlSO4+	1.300e-30	1.039e-30	-29.886	-29.983	-0.097
Al+3	3.784e-31	7.731e-32	-30.422	-31.112	-0.690
Al(SO4)2-	1.839e-31	1.470e-31	-30.735	-30.833	-0.097
AlF6-3	2.986e-33	3.969e-34	-32.525	-33.401	-0.876
AlHSO4+2	0.000e+00	0.000e+00	-43.107	-43.496	-0.389
B	2.135e-05				
H2BO3-	2.133e-05	1.705e-05	-4.671	-4.768	-0.097
H3BO3	1.182e-08	1.203e-08	-7.927	-7.920	0.008
BF(OH)3-	8.524e-13	6.812e-13	-12.069	-12.167	-0.097
BF2(OH)2-	5.078e-21	4.058e-21	-20.294	-20.392	-0.097
BF3OH-	3.435e-31	2.745e-31	-30.464	-30.561	-0.097
BF4-	0.000e+00	0.000e+00	-40.109	-40.206	-0.097
Ba	2.338e-06				

	Ba+2	1.088e-06	4.509e-07	-5.963	-6.346	-0.383
	BaSO4	1.022e-06	1.040e-06	-5.991	-5.983	0.008
	BaCO3	1.748e-07	1.778e-07	-6.758	-6.750	0.008
	BaOH+	5.257e-08	4.201e-08	-7.279	-7.377	-0.097
	BaHCO3+	3.402e-11	2.719e-11	-10.468	-10.566	-0.097
Br		3.641e-05				
	Br-	3.641e-05	2.831e-05	-4.439	-4.548	-0.109
C(4)		7.399e-03				
	CaCO3	5.069e-03	5.158e-03	-2.295	-2.288	0.008
	CO3-2	2.035e-03	8.612e-04	-2.691	-3.065	-0.373
	NaCO3-	2.775e-04	2.217e-04	-3.557	-3.654	-0.097
	HCO3-	9.421e-06	7.599e-06	-5.026	-5.119	-0.093
	SrCO3	7.541e-06	7.673e-06	-5.123	-5.115	0.008
	CaHCO3+	4.297e-07	3.466e-07	-6.367	-6.460	-0.093
	MgCO3	2.188e-07	2.227e-07	-6.660	-6.652	0.008
	BaCO3	1.748e-07	1.778e-07	-6.758	-6.750	0.008
	NaHCO3	7.908e-08	8.047e-08	-7.102	-7.094	0.008
	SrHCO3+	1.955e-09	1.577e-09	-8.709	-8.802	-0.093
	BaHCO3+	3.402e-11	2.719e-11	-10.468	-10.566	-0.097
	MgHCO3+	3.231e-11	2.582e-11	-10.491	-10.588	-0.097
	CO2	6.646e-12	6.763e-12	-11.177	-11.170	0.008
	Pb(CO3)2-2	1.269e-13	5.175e-14	-12.897	-13.286	-0.389
	PbCO3	2.351e-14	2.392e-14	-13.629	-13.621	0.008
	PbHCO3+	1.207e-20	9.648e-21	-19.918	-20.016	-0.097
Ca		2.003e-02				
	Ca+2	9.304e-03	3.967e-03	-2.031	-2.402	-0.370
	CaCO3	5.069e-03	5.158e-03	-2.295	-2.288	0.008
	CaSO4	3.381e-03	3.440e-03	-2.471	-2.463	0.008
	CaOH+	2.265e-03	1.810e-03	-2.645	-2.742	-0.097
	CaF+	5.685e-06	4.543e-06	-5.245	-5.343	-0.097
	CaHCO3+	4.297e-07	3.466e-07	-6.367	-6.460	-0.093
	CaPO4-	2.115e-07	1.690e-07	-6.675	-6.772	-0.097
	CaHPO4	2.860e-11	2.911e-11	-10.544	-10.536	0.008
	CaHSO4+	8.534e-15	6.820e-15	-14.069	-14.166	-0.097
	CaH2PO4+	1.025e-17	8.192e-18	-16.989	-17.087	-0.097
Cl		1.755e-03				
	Cl-	1.755e-03	1.380e-03	-2.756	-2.860	-0.104
	PbCl+	9.439e-20	7.543e-20	-19.025	-19.122	-0.097
	PbCl2	1.817e-22	1.849e-22	-21.741	-21.733	0.008
	PbCl3-	2.442e-25	1.952e-25	-24.612	-24.710	-0.097
	PbCl4-2	3.014e-28	1.229e-28	-27.521	-27.910	-0.389
F		2.007e-04				
	F-	1.934e-04	1.517e-04	-3.714	-3.819	-0.106
	CaF+	5.685e-06	4.543e-06	-5.245	-5.343	-0.097
	NaF	1.615e-06	1.643e-06	-5.792	-5.784	0.008
	MgF+	3.335e-09	2.665e-09	-8.477	-8.574	-0.097
	BF(OH)3-	8.524e-13	6.812e-13	-12.069	-12.167	-0.097
	HF	7.295e-14	7.423e-14	-13.137	-13.129	0.008
	HF2-	5.136e-17	4.105e-17	-16.289	-16.387	-0.097
	BF2(OH)2-	5.078e-21	4.058e-21	-20.294	-20.392	-0.097
	AlF3	1.552e-26	1.579e-26	-25.809	-25.802	0.008
	AlF2+	1.041e-26	8.321e-27	-25.982	-26.080	-0.097
	AlF4-	1.191e-27	9.520e-28	-26.924	-27.021	-0.097
	AlF+2	2.771e-28	1.130e-28	-27.557	-27.947	-0.389
	AlF5-2	5.681e-30	2.317e-30	-29.246	-29.635	-0.389
	BF3OH-	3.435e-31	2.745e-31	-30.464	-30.561	-0.097
	AlF6-3	2.986e-33	3.969e-34	-32.525	-33.401	-0.876

	BF4-	0.000e+00	0.000e+00	-40.109	-40.206	-0.097
	SiF6-2	0.000e+00	0.000e+00	-48.644	-49.033	-0.389
H(0)		1.950e-36				
	H2	9.748e-37	9.919e-37	-36.011	-36.004	0.008
K		8.980e-03				
	K+	8.669e-03	6.817e-03	-2.062	-2.166	-0.104
	KSO4-	2.479e-04	1.981e-04	-3.606	-3.703	-0.097
	KOH	6.387e-05	6.500e-05	-4.195	-4.187	0.008
	KHPO4-	2.496e-13	1.994e-13	-12.603	-12.700	-0.097
Mg		3.301e-06				
	MgOH+	2.136e-06	1.707e-06	-5.670	-5.768	-0.097
	Mg+2	6.745e-07	2.971e-07	-6.171	-6.527	-0.356
	MgSO4	2.691e-07	2.738e-07	-6.570	-6.563	0.008
	MgCO3	2.188e-07	2.227e-07	-6.660	-6.652	0.008
	MgF+	3.335e-09	2.665e-09	-8.477	-8.574	-0.097
	MgHCO3+	3.231e-11	2.582e-11	-10.491	-10.588	-0.097
	MgPO4-	2.137e-11	1.708e-11	-10.670	-10.768	-0.097
	MgHPO4	2.897e-15	2.948e-15	-14.538	-14.531	0.008
	MgH2PO4+	9.778e-22	7.814e-22	-21.010	-21.107	-0.097
N(5)		1.540e-03				
	NO3-	1.540e-03	1.198e-03	-2.812	-2.922	-0.109
	PbNO3+	3.543e-20	2.831e-20	-19.451	-19.548	-0.097
Na		2.465e-02				
	Na+	2.351e-02	1.883e-02	-1.629	-1.725	-0.096
	NaSO4-	5.228e-04	4.178e-04	-3.282	-3.379	-0.097
	NaOH	3.362e-04	3.421e-04	-3.473	-3.466	0.008
	NaCO3-	2.775e-04	2.217e-04	-3.557	-3.654	-0.097
	NaF	1.615e-06	1.643e-06	-5.792	-5.784	0.008
	NaHCO3	7.908e-08	8.047e-08	-7.102	-7.094	0.008
	NaHPO4-	6.894e-13	5.509e-13	-12.162	-12.259	-0.097
O(0)		8.770e-23				
	O2	4.385e-23	4.462e-23	-22.358	-22.350	0.008
P		2.117e-07				
	CaPO4-	2.115e-07	1.690e-07	-6.675	-6.772	-0.097
	PO4-3	1.365e-10	1.648e-11	-9.865	-10.783	-0.918
	HPO4-2	3.839e-11	1.500e-11	-10.416	-10.824	-0.408
	CaHPO4	2.860e-11	2.911e-11	-10.544	-10.536	0.008
	MgPO4-	2.137e-11	1.708e-11	-10.670	-10.768	-0.097
	NaHPO4-	6.894e-13	5.509e-13	-12.162	-12.259	-0.097
	KHPO4-	2.496e-13	1.994e-13	-12.603	-12.700	-0.097
	MgHPO4	2.897e-15	2.948e-15	-14.538	-14.531	0.008
	H2PO4-	1.140e-16	9.080e-17	-15.943	-16.042	-0.099
	CaH2PO4+	1.025e-17	8.192e-18	-16.989	-17.087	-0.097
	MgH2PO4+	9.778e-22	7.814e-22	-21.010	-21.107	-0.097
Pb		4.842e-08				
	Pb(OH) 4-2	4.471e-08	1.824e-08	-7.350	-7.739	-0.389
	Pb(OH) 3-	3.622e-09	2.895e-09	-8.441	-8.538	-0.097
	Pb(OH) 2	9.010e-11	9.169e-11	-10.045	-10.038	0.008
	Pb(CO3) 2-2	1.269e-13	5.175e-14	-12.897	-13.286	-0.389
	PbOH+	1.072e-13	8.570e-14	-12.970	-13.067	-0.097
	PbCO3	2.351e-14	2.392e-14	-13.629	-13.621	0.008
	PbSO4	4.065e-18	4.136e-18	-17.391	-17.383	0.008
	Pb+2	3.919e-18	1.598e-18	-17.407	-17.796	-0.389
	Pb(SO4) 2-2	2.449e-19	9.990e-20	-18.611	-19.000	-0.389
	PbCl+	9.439e-20	7.543e-20	-19.025	-19.122	-0.097
	PbNO3+	3.543e-20	2.831e-20	-19.451	-19.548	-0.097
	PbHCO3+	1.207e-20	9.648e-21	-19.918	-20.016	-0.097

	PbCl2	1.817e-22	1.849e-22	-21.741	-21.733	0.008
	PbCl3-	2.442e-25	1.952e-25	-24.612	-24.710	-0.097
	PbCl4-2	3.014e-28	1.229e-28	-27.521	-27.910	-0.389
	Pb2OH+3	2.307e-29	3.067e-30	-28.637	-29.513	-0.876
S(6)		1.535e-02				
	SO4-2	1.119e-02	4.602e-03	-1.951	-2.337	-0.386
	CaSO4	3.381e-03	3.440e-03	-2.471	-2.463	0.008
	NaSO4-	5.228e-04	4.178e-04	-3.282	-3.379	-0.097
	KSO4-	2.479e-04	1.981e-04	-3.606	-3.703	-0.097
	SrSO4	1.367e-05	1.391e-05	-4.864	-4.857	0.008
	BaSO4	1.022e-06	1.040e-06	-5.991	-5.983	0.008
	MgSO4	2.691e-07	2.738e-07	-6.570	-6.563	0.008
	HSO4-	1.789e-13	1.430e-13	-12.747	-12.845	-0.097
	CaHSO4+	8.534e-15	6.820e-15	-14.069	-14.166	-0.097
	PbSO4	4.065e-18	4.136e-18	-17.391	-17.383	0.008
	Pb(SO4)2-2	2.449e-19	9.990e-20	-18.611	-19.000	-0.389
	AlSO4+	1.300e-30	1.039e-30	-29.886	-29.983	-0.097
	Al(SO4)2-	1.839e-31	1.470e-31	-30.735	-30.833	-0.097
	AlHSO4+2	0.000e+00	0.000e+00	-43.107	-43.496	-0.389
Si		8.349e-05				
	H3SiO4-	6.694e-05	5.350e-05	-4.174	-4.272	-0.097
	H2SiO4-2	1.639e-05	6.685e-06	-4.785	-5.175	-0.389
	H4SiO4	1.608e-07	1.637e-07	-6.794	-6.786	0.008
	SiF6-2	0.000e+00	0.000e+00	-48.644	-49.033	-0.389
Sr		6.298e-05				
	Sr+2	3.883e-05	1.666e-05	-4.411	-4.778	-0.367
	SrSO4	1.367e-05	1.391e-05	-4.864	-4.857	0.008
	SrCO3	7.541e-06	7.673e-06	-5.123	-5.115	0.008
	SrOH+	2.929e-06	2.350e-06	-5.533	-5.629	-0.096
	SrHCO3+	1.955e-09	1.577e-09	-8.709	-8.802	-0.093

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

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-4.99	6.21	11.20	Al(OH)3
Albite	-8.34	-3.43	4.91	NaAlSi3O8
Alunite	-24.90	-25.54	-0.64	KAl3(SO4)2(OH)6
Anglesite	-12.31	-20.13	-7.82	PbSO4
Anhydrite	-0.40	-4.74	-4.34	CaSO4
Anorthite	-5.40	21.32	26.72	CaAl2Si2O8
Aragonite	2.83	-5.47	-8.30	CaCO3
Barite	1.39	-8.68	-10.07	BaSO4
Ca-Montmorillonite	-15.12	-6.73	8.39	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	2.98	-5.47	-8.45	CaCO3
Celestite	-0.49	-7.12	-6.62	SrSO4
Cerrusite	-7.66	-20.86	-13.20	PbCO3
Chalcedony	-3.16	-6.78	-3.62	SiO2
Chlorite(14A)	13.16	83.82	70.66	Mg5Al2Si3O10(OH)8
Chrysotile	8.53	41.49	32.96	Mg3Si2O5(OH)4
CO2(g)	-9.78	-27.94	-18.17	CO2
Dolomite	1.89	-15.06	-16.95	CaMg(CO3)2
Fluorite	0.63	-10.04	-10.67	CaF2
Gibbsite	-2.25	6.21	8.45	Al(OH)3
Gypsum	-0.16	-4.74	-4.58	CaSO4·2H2O
H2(g)	-32.88	-32.88	0.00	H2
Hydroxyapatite	8.16	-31.92	-40.07	Ca5(PO4)3OH

Illite	-11.23	1.28	12.51	K _{0.6} Mg _{0.25} Al _{2.3} Si _{3.5} O ₁₀ (OH) ₂
K-feldspar	-6.14	-3.87	2.27	KAlSi ₃ O ₈
K-mica	-5.06	8.54	13.60	KAl ₃ Si ₃ O ₁₀ (OH) ₂
Kaolinite	-9.12	-1.16	7.97	Al ₂ Si ₂ O ₅ (OH) ₄
O ₂ (g)	-19.42	65.76	85.18	O ₂
Pb(OH) ₂	-1.28	7.08	8.36	Pb(OH) ₂
Quartz	-2.71	-6.78	-4.07	SiO ₂
Sepiolite	0.43	16.35	15.92	Mg ₂ Si ₃ O ₇ .5OH:3H ₂ O
Sepiolite(d)	-2.31	16.35	18.66	Mg ₂ Si ₃ O ₇ .5OH:3H ₂ O
SiO ₂ (a)	-4.02	-6.78	-2.76	SiO ₂
Strontianite	1.43	-7.84	-9.27	SrCO ₃
Talc	5.82	27.92	22.10	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Witherite	-0.83	-9.41	-8.58	BaCO ₃

 End of simulation.

 Reading input data for simulation 2.

 End of run.
