THE CONTENTS OF THIS SECTION ARE
THE HIGHEST QUALITY AVAILABLE

INITIAL [illegible] DATE 9/27/02

PAGE NUMBERING SEQUENCE IS INCONSISTENT

Appendix A

Constituent Solubility Modeled Using PHREEQC

Table A-1. Constituents considered significantly Leachable (Kd <20).

Constituent	Kd (L/kg)	Reference
1,1,1-Trichloroethane	0.41	1
1,1,2,2-Tetrachloroethane	0.24	1
1,1,2-Trichloroethane	0.23	1
1,1-Dichloroethane	0.16	1
1,1-Dichloroethene	0.20	1
1,2,4-Trichlorobenzene	4.98	1
1,2-Dichlorobenzene	1.14	1
1,2-Dichloroethane	0.11	1
1,2-Dichloroethene (total)	0.11	1
1,3-Dichlorobenzene	4.44	2
1,4-Dichlorobenzene	1.85	1
1,4-Dioxane	0.00	2
2,4,5-Trichlorophenol	2.12	2
2,4,6-Trichlorophenol	7.54	2
2,4-Dichlorophenol	1.04	2
2,4-Dimethylphenol	0.63	1
2,4-Dinitrophenol	0.06	2
2,4-Dinitrotoluene	0.29	1
2,6-Dinitrotoluene	0.21	1
2-Butanone	0.04	2
2-Chlorophenol	0.26	2
2-Hexanone	0.04	2
2-Methylnaphthalene	unknown	none
2-Methylphenol	0.27	1
2-Nitroaniline	0.05	2
2-Nitrophenol	0.13	2
3,3'-Dichlorobenzidine	1.94	2
3-Methyl Butanal	unknown	none
3-Nitroaniline	0.04	2
4,6-Dinitro-2-methylphenol	unknown	none
4-Chloro-3-methylphenol	2.33	2
4-Chloroaniline	0.13	2
4-Methyl-2-Pentanone	unknown	none
4-Methylphenol	0.02	2
4-Nitroaniline	unknown	none
4-Nitrophenol	0.15	2
Acenaphthene	14.69	1
Acetone	0.00	1
Acetonitrile	0.00	2
Acrolein	0.00	2
Acrylonitrile	0.00	2
Aramite	unknown	none
As	3.00	1
At	0.00	1
B	5.00	1
Benzene	0.19	1
Benzidine	0.04	2
Benzoic acid	0.14	2
bis(2-Chloroethoxy)methane	0.01	2
bis(2-Chloroethyl)ether	0.23	1

Table A-1. Constituents considered significantly Leachable (Kd <20).

Constituent	Kd (L/kg)	Reference
bis(2-Chloroisopropyl)ether	0.70	2
bis(2-Ethylhexyl)phthalate	18.00	1
Butane,1,1,3,4-Tetrachloro-	unknown	none
C-14	5.00	1
Ca	5.00	1
Carbazole	10.17	1
Carbon Disulfide	0.14	1
Cd	6.00	1
Chlorobenzene	0.67	1
Chloroethane	0.05	2
Chloromethane	0.02	2
Cl	0.00	1
Co	10.00	1
Cu	20.00	1
Cyanide	0.00	1
Decane, 3,4-Dimethyl	unknown	none
Diacetone alcohol	unknown	none
Dibenzofuran	unknown	none
Diethylphthalate	0.25	1
Dimethyl Disulfide	0.11	2
Dimethylphthalate	0.07	2
Di-n-butylphthalate	4.70	1
Eicosane	unknown	none
Ethyl cyanide	unknown	none
Ethylbenzene	0.61	1
Famphur	unknown	none
Fluoride	0.00	1
Heptadecane, 2,6,10,15-Tetra	unknown	none
Hexachlorobutadiene	10.17	2
Hexachloroethane	5.34	1
I	0.00	1
Isobutyl alcohol	unknown	none
Isophorone	0.14	1
Isopropyl Alcohol/2-propanol	unknown	none
K	15.00	1
Kepone	unknown	none
Kr	0.00	1
Mesityl oxide	unknown	none
Methyl Acetate	0.00	2
Methylene Chloride	0.03	1
Mg	5.00	1
Mo	10.00	1
Naphthalene	3.57	1
Nitrate	0.00	1
Nitrate/Nitrite-N	0.00	1
Nitrite	0.00	1
Nitrobenzene	0.36	1
N-Nitroso-di-n-propylamine	0.07	1
N-Nitrosodiphenylamine	3.87	1
Np	8.00	1

Table A-1. Constituents considered significantly Leachable (Kd <20).

Constituent	Kd (L/kg)	Reference
Octane,2,3,7-Trimethyl	unknown	none
o-Toluenesulfonamide	unknown	none
P	5.00	1
Phenol	0.09	1
Phenol,2,6-Bis(1,1-Dimethyl)	unknown	none
p-Toluenesulfonamide	unknown	none
Rn	0.00	1
Se	4.00	1
Styrene	2.74	1
Sulfate	14.00	1
Sulfide	14.00	1
Tc	0.20	1
Tetrachloroethene	0.80	1
Toluene	1.00	1
Tributylphosphate	unknown	none
Trichloroethene	0.28	1
Tritium	0.00	1
U	6.00	1
Undecane,4,6-Dimethyl-	unknown	none
V	6.00	1
Xe	0.00	1
Xylene (ortho)	0.72	1
Xylene (total)	0.59	1
Zn	16.00	1

References:

1= Jenkins, T., DOE, letter to Martin Doornbos, BBWI, July 3, 2001, *Kd values for INTEC groundwater modeling* (EM-ER-01-115).

2= Verschueren, Karel, 1983, Handbook of Environmental Data on Organic Chemicals, Second Edition, Van Nostrand Reinhold pub. New York, New York, and Callahan, et.al, 1979, Water -Related Environmental Fate of 123 Priority Pollutants, EPA-440/4-79-029 a and b.

Table A-2. Constituents not considered significantly leachable (Kd>20 L/kg).

Constituent	Kd (L/kg)	Reference
2-Chloronaphthalene	2.44E+01	2
4-Bromophenyl-phenylether	3.52E+01	2
4-Chlorophenyl-phenylether	2.22E+01	2
Ac	4.50E+02	1
Acenaphthylene	2.17E+01	2
Ag	9.00E+01	1
Al	2.50E+02	1
Am	3.40E+02	1
Anthracene	7.05E+01	1
Aroclor-1016	1.00E+02	1
Aroclor-1254	1.00E+02	1
Aroclor-1260	1.00E+02	1
Aroclor-1268	1.00E+02	1
Ba	5.00E+01	1
Be	2.50E+02	1
Benzo(a)anthracene	1.07E+03	1
Benzo(a)pyrene	1.20E+03	1
Benzo(b)fluoranthene	3.69E+03	1
Benzo(g,h,i)perylene	3.14E+04	2
Benzo(k)fluoranthene	3.69E+03	1
Bi	1.00E+02	1
Bk	4.00E+03	1
Butylbenzylphthalate	4.12E+01	1
Ce	5.00E+02	1
Cf	5.10E+02	1
Chrysene	1.19E+03	1
Cm	4.00E+03	1
Cr	3.00E+01	1
Cs	5.00E+02	1
Dibenz(a,h)anthracene	5.37E+03	1
Di-n-octylphthalate	2.50E+05	1
Dysprosium	2.40E+02	1
Er	2.40E+02	1
Eu	2.40E+02	1
Fe	2.20E+02	1
Fluoranthene	1.47E+02	1
Fluorene	2.31E+01	1
Fr	5.00E+02	1
Gd	2.40E+02	1
Hexachlorobenzene	2.40E+02	1
Hexachlorocyclopentadiene	6.00E+02	1
Hf	4.50E+02	1
Hg	1.00E+02	1
Ho	2.50E+02	1
In	3.90E+02	1
Indeno(1,2,3-cd)pyrene	1.04E+04	1
La	1.20E+03	1
Mn	5.00E+01	1
Na	7.60E+01	1
Nb	1.60E+02	1

Table A-2. Constituents not considered significantly leachable (Kd>20 L/kg).

Constituent	Kd (L/kg)	Reference
Nd	2.40E+02	1
Ni	1.00E+02	1
Pa	5.50E+02	1
Pb	1.00E+02	1
Pd	5.50E+01	1
Pentachlorophenol	2.38E+03	2
Phenanthrene	1.89E+02	2
Pm	2.40E+02	1
Po	1.50E+02	1
Pr	2.40E+02	1
Pu	1.40E+02	1
Pyrene	2.04E+02	1
Ra	1.00E+02	1
Rb	5.50E+01	1
Ru	5.50E+01	1
Sb	5.00E+01	1
Sc	3.10E+02	1
Sm	2.45E+02	1
Sn	1.30E+02	1
Sr	2.40E+01	1
Ta	2.20E+02	1
Tb	2.40E+02	1
Te	1.25E+02	1
Th	1.00E+02	1
Tl	1.00E+02	1
Tm	2.40E+02	1
Y	1.70E+02	1
Zr	6.00E+02	1

References:

1= Jenkins, T., DOE, letter to Martin Doornbos, BBWI, July 3, 2001, *Kd values for INTEC groundwater modeling* (EM-ER-01-115).

2= Verschueren, Karel, 1983, Handbook of Environmental Data on Organic Chemicals, Second Edition, Van Nostrand Reinhold pub. New York, New York, and Callahan, et.al, 1979, Water -Related Environmental Fate of 123 Priority Pollutants, EPA-440/4-79-029 a and b.

Table A-3. Screened constituents used in geochemical modeling.

Cations	Element	Symbol	Element Quantity from Design Inventory (kg)	Percent of Total Design Inventory Mass (a)
	Calcium	Ca	1.24E+07	2.12E+00
	Iron	Fe	6.00E+06	1.03E+00
	Aluminum	Al	4.16E+06	7.11E-01
	Magnesium	Mg	2.62E+06	4.48E-01
	Potassium	K	6.73E+05	1.15E-01
	Terbium	Tb	3.35E+05	5.73E-02
	Sodium	Na	1.25E+05	2.14E-02
	Zinc	Zn	1.22E+05	2.08E-02
	Manganese	Mn	1.21E+05	2.06E-02
	Ytterbium	Yb	1.14E+05	1.95E-02
	Barium	Ba	1.06E+05	1.80E-02
Anions (b)	Carbon (rad)	C	4.90E-09	N/A (c)
	Iodine (rad)	I	4.30E+00	N/A (c)
	Technitium (rad)	Tc	1.99E-01	N/A (c)
	Tellurium (rad)	Te	1.13E-08	N/A (c)
	Plutonium (rad)	Pu	7.50E-02	N/A (c)
	Uranium (rad)	U	3.47E+03	N/A (c)
	Phosphorus	P	5.70E+04	N/A (c)
	Vanadium	V	1.26E+04	N/A (c)
	Sulfate	SO4	1.20E+04	N/A (c)
	Arsenic	As	3.33E+03	N/A (c)
	Nitrate	NO3	2.30E+03	N/A (c)
	Fluoride	F	2.26E+03	N/A (c)
	Chloride	Cl	1.09E+03	N/A (c)
	Selenium	Se	4.99E+02	N/A (c)
	Cyanide	CN	1.97E+02	N/A (c)
	Nitrite	NO2	4.97E+00	N/A (c)
	Boron	B	1.08E+05	N/A (c)
	Sulfide	S	4.44E+05	N/A (c)

Notes:

(a) Calculated by dividing the kg of each constituent by 5.85E+08 kg, the total inventory mass.

(b) Radioactive anions expressed as total mass of all reported isotopes

(c) Anions were not screened on the basis of percentage of total inventory mass.

Table A-4. Organic and cationic constituents eliminated during screening process (1).

Organics	Constituent	kg	% of total
	1,1,1-Trichloroethane	7.43E+00	1.27E-06
	1,1,2,2-Tetrachloroethane	2.34E-02	4.01E-09
	1,1,2-Trichloroethane	1.15E-01	1.96E-08
	1,1-Dichloroethane	1.11E+00	1.89E-07
	1,1-Dichloroethene	7.01E-01	1.20E-07
	1,2,4-Trichlorobenzene	5.39E+00	9.21E-07
	1,2-Dichlorobenzene	5.39E+00	9.21E-07
	1,2-Dichloroethane	2.55E-03	4.36E-10
	1,2-Dichloroethene (total)	1.54E-01	2.62E-08
	1,3-Dichlorobenzene	5.39E+00	9.21E-07
	1,4-Dichlorobenzene	2.13E+02	3.64E-05
	1,4-Dioxane	8.91E-03	1.52E-09
	2,4,5-Trichlorophenol	2.11E+01	3.61E-06
	2,4,6-Trichlorophenol	8.65E+00	1.48E-06
	2,4-Dichlorophenol	1.02E+01	1.75E-06
	2,4-Dimethylphenol	8.65E+00	1.48E-06
	2,4-Dinitrophenol	2.41E+01	4.12E-06
	2,4-Dinitrotoluene	5.39E+00	9.21E-07
	2,6-Dinitrotoluene	9.80E+00	1.67E-06
	2-Butanone	1.17E+01	2.00E-06
	2-Chloronaphthalene	5.39E+00	9.21E-07
	2-Chlorophenol	8.65E+00	1.48E-06
	2-Hexanone	1.28E+00	2.18E-07
	2-Methylnaphthalene	2.42E+02	4.14E-05
	2-Methylphenol	9.78E+00	1.67E-06
	2-Nitroaniline	1.29E+01	2.20E-06
	2-Nitrophenol	8.65E+00	1.48E-06
	3,3'-Dichlorobenzidine	5.39E+00	9.21E-07
	3-Methyl Butanal	1.06E-01	1.81E-08
	3-Nitroaniline	1.29E+01	2.20E-06
	4,6-Dinitro-2-methylphenol	2.11E+01	3.61E-06
	4-Bromophenyl-phenylether	5.39E+00	9.21E-07
	4-Chloro-3-methylphenol	8.65E+00	1.48E-06
	4-Chloroaniline	1.93E+01	3.30E-06
	4-Chlorophenyl-phenylether	5.39E+00	9.21E-07
	4-Methyl-2-Pentanone	1.40E+01	2.40E-06
	4-Methylphenol	1.83E+01	3.12E-06
	4-Nitroaniline	1.29E+01	2.20E-06
	4-Nitrophenol	2.44E+01	4.17E-06
	Acenaphthene	9.58E+01	1.64E-05
	Acenaphthylene	9.80E+00	1.67E-06
	Acetone	2.94E+02	5.02E-05
	Acetonitrile	8.91E-03	1.52E-09
	Acrolein	4.29E-03	7.33E-10
	Acrylonitrile	4.29E-03	7.33E-10
	Anthracene	1.52E+02	2.59E-05
	Aramite	5.42E-02	9.27E-09
	Aroclor-1016	3.64E+00	6.22E-07

Table A-4. Organic and cationic constituents eliminated during screening process (1).

Organics	Constituent	kg	% of total
	Aroclor-1254	6.08E+01	1.04E-05
	Aroclor-1260	3.41E+02	5.84E-05
	Aroclor-1268	2.94E+01	5.03E-06
	Benzene	2.86E+02	4.89E-05
	Benzidine	1.38E-01	2.35E-08
	Benzo(a)anthracene	1.20E+02	2.05E-05
	Benzo(a)pyrene	4.97E+01	8.49E-06
	Benzo(b)fluoranthene	8.50E+01	1.45E-05
	Benzo(g,h,i)perylene	5.39E+00	9.21E-07
	Benzo(k)fluoranthene	8.81E+00	1.51E-06
	Benzoic acid	4.05E+00	6.93E-07
	bis(2-Chloroethoxy)methane	5.39E+00	9.21E-07
	bis(2-Chloroethyl)ether	5.39E+00	9.21E-07
	bis(2-Chloroisopropyl)ether	5.39E+00	9.21E-07
	bis(2-Ethylhexyl)phthalate	6.97E+01	1.19E-05
	Butane,1,1,3,4-Tetrachloro-	3.74E+00	6.39E-07
	Butylbenzylphthalate	3.22E+01	5.50E-06
	Carbazole	1.53E+01	2.62E-06
	Carbon Disulfide	2.16E+01	3.69E-06
	Chlorobenzene	3.11E+00	5.32E-07
	Chloroethane	1.43E-03	2.44E-10
	Chloromethane	1.67E-01	2.86E-08
	Chrysene	1.26E+02	2.15E-05
	Decane, 3,4-Dimethyl	7.64E-02	1.31E-08
	Diacetone alcohol	2.05E+03	3.50E-04
	Dibenz(a,h)anthracene	5.39E+00	9.21E-07
	Dibenzofuran	1.54E+02	2.62E-05
	Diethylphthalate	5.39E+00	9.22E-07
	Dimethyl Disulfide	1.40E+00	2.40E-07
	Dimethylphthalate	5.39E+00	9.21E-07
	Di-n-butylphthalate	1.13E+01	1.93E-06
	Di-n-octylphthalate	1.24E+01	2.12E-06
	Eicosane	1.34E+00	2.29E-07
	Ethyl cyanide	8.91E-03	1.52E-09
	Ethylbenzene	3.70E+01	6.32E-06
	Famphur	2.75E-02	4.71E-09
	Fluoranthene	3.61E+02	6.17E-05
	Fluorene	8.70E+01	1.49E-05
	Heptadecane, 2,6,10,15-Tetra	1.63E+00	2.78E-07
	Hexachlorobenzene	5.39E+00	9.21E-07
	Hexachlorobutadiene	9.80E+00	1.67E-06
	Hexachlorocyclopentadiene	5.39E+00	9.21E-07
	Hexachloroethane	5.39E+00	9.21E-07
	Indeno(1,2,3-cd)pyrene	5.39E+00	9.21E-07
	Isobutyl alcohol	8.91E-03	1.52E-09
	Isophorone	5.39E+00	9.22E-07
	Isopropyl Alcohol/2-propanol	1.01E+00	1.72E-07
	Kepone	4.70E+01	8.03E-06

Table A-4. Organic and cationic constituents eliminated during screening process (1).

Organics	Constituent	kg	% of total
	Mesityl oxide	4.01E+01	6.86E-06
	Methyl Acetate	2.29E-01	3.92E-08
	Methylene Chloride	3.96E+01	6.77E-06
	Naphthalene	2.01E+02	3.44E-05
	Nitrobenzene	5.39E+00	9.21E-07
	N-Nitroso-di-n-propylamine	5.39E+00	9.21E-07
	N-Nitrosodiphenylamine	5.39E+00	9.21E-07
	Octane,2,3,7-Trimethyl	7.64E-02	1.31E-08
	o-Toluenesulfonamide	2.40E+00	4.09E-07
	Pentachlorophenol	2.65E+01	4.53E-06
	Phenanthrene	5.53E+02	9.46E-05
	Phenol	3.78E+01	6.46E-06
	Phenol,2,6-Bis(1,1-Dimethyl)	1.92E+00	3.28E-07
	p-Toluenesulfonamide	2.40E+00	4.09E-07
	Pyrene	1.20E+02	2.05E-05
	Styrene	4.86E-04	8.30E-11
	Tetrachloroethene	4.56E+00	7.80E-07
	Toluene	4.65E+02	7.95E-05
	Tributylphosphate	1.72E+02	2.94E-05
	Trichloroethene	3.41E+01	5.83E-06
	Undecane,4,6-Dimethyl-	7.64E-02	1.31E-08
	Xylene (ortho)	1.84E+00	3.14E-07
	Xylene (total)	1.64E+03	2.80E-04
Cations		kg	% of total
	Antimony	3.41E+03	5.83E-04
	Arsenic	3.33E+03	5.69E-04
	Beryllium	1.70E+02	2.90E-05
	Cadmium	2.11E+03	3.60E-04
	Chloride	1.09E+03	1.87E-04
	Chromium	2.41E+04	4.13E-03
	Cobalt	3.53E+03	6.03E-04
	Copper	1.75E+04	2.99E-03
	Cyanide	1.97E+02	3.37E-05
	Dysprosium	3.47E+04	5.93E-03
	Fluoride	2.26E+03	3.87E-04
	Lead	3.38E+04	5.77E-03
	Mercury	5.53E+03	9.45E-04
	Molybdenum	5.95E+03	1.02E-03
	Nickel	1.15E+04	1.97E-03
	Nitrate	2.30E+03	3.93E-04
	Nitrate/Nitrite-N	1.30E+02	2.22E-05
	Nitrite	4.97E+00	8.49E-07
	Phosphorus	5.70E+04	9.74E-03
	Selenium	4.99E+02	8.52E-05
	Silver	5.75E+03	9.84E-04
	Strontium	1.06E+04	1.82E-03
	Sulfate	1.20E+04	2.05E-03

Table A-4. Organic and cationic constituents eliminated during screening process (1).

Organics	Constituent	kg	% of total
	Thallium	2.17E+02	3.70E-05
	Vanadium	1.26E+04	2.15E-03
	Zirconium	4.04E+04	6.91E-03

Notes

(1) Criterion for organics to be included was a mass concentration greater than 1% of total waste mass; criterion for cations to be included was a mass concentration greater than 0.01% of total waste mass; Total waste mass assumed to be 5.85E+08 kg.

Table A-5. Quantities of mineral phases used in geochemical modeling.

Constituent [a]	Chemical Formula	Constituent Molar Mass (g/mol)	Mass Concentration from Design Inventory (mg/kg)[b]	Moles of Constituent per kg	Mineral Source(s)	Moles of Mineral Sources Exposed to 1L Leachate[c]	Mineral(s) Controlling Solubility
Aluminum	Al	27.0	7.11E+03	2.64E-01	Albite (NaAlSi3O8), Orthoclase (KAlSi3O8), Illite (K0.6Mg0.25Al2.3Si3.5O10(OH)2)	14, 7.8, 4.1[d]	Kaolinite (Al2Si2O5(OH)4)
Arsenic	As	74.9	5.69E+00	7.59E-05	Ca3(AsO4)2	6E-04	none
Barium	Ba	137.0	1.80E+02	1.32E-03	Barite (BaSO4)	2E-02	Barite (BaSO4)
Boron	B	10.8	1.85E+02	1.71E-02	Borax (Na2B4O5(OH)4.8H2O)	7E-02	Borax (Na2B4O5(OH)4.8H2O)
Calcium	Ca	40.0	2.12E+04	5.30E-01	Calcite (CaCO3)	6.1[d]	Calcite (CaCO3)
Carbon (rad)	C	14.0	1.03E-11	7.39E-16	not considered[e]	not considered[e]	not considered[e]
Chloride	Cl	35.5	1.87E+00	5.26E-05	Halite (NaCl)	9E-04	none
Cyanide	CN	26.0	3.37E-01	1.29E-05	NaCN	2.16E-04	oxidized to NO3
Fluoride	F	19.0	3.87E+00	2.03E-04	Fluoroapatite (Ca5(PO4)3F)	3E-03	Fluoroapatite (Ca5(PO4)3F)
Iodine (rad)	I	129.0	7.35E-03	5.70E-08	NaI	9.49E-07	none
Iron	Fe	55.8	1.03E+04	1.84E-01	Fe(OH)3, pyrite (FeS2)	2.9, 0.17	Fe(OH)3
Magnesium	Mg	24.3	4.48E+03	1.84E-01	Enstatite (MgSiO3), Illite (K0.6Mg0.25Al2.3Si3.5O10(OH)2)	22, 4.1[d]	dolomite
Manganese	Mn	54.9	2.06E+02	3.76E-03	Birnessite (Mn8O14.5H2O)	8E-03	Birnessite (Mn8O14.5H2O)
Nitrate	NO3	62.0	3.93E+00	6.33E-05	Niter (KNO3)	1E-03	none
Nitrite	NO2	46.0	8.49E-03	1.84E-07	not considered[f]	not considered[f]	oxidized to NO3
Phosphorus	P	31.0	9.74E+01	3.14E-03	Fluoroapatite (Ca5(PO4)3F)	2E-02	Fluoroapatite (Ca5(PO4)3F)
Plutonium (rad)	Pu	244.0	1.28E-04	5.26E-10	PuO2	8.76E-09	PuO2
Potassium	K	39.1	1.15E+03	2.94E-02	Orthoclase (KAlSi3O8), Illite (K0.6Mg0.25Al2.3Si3.5O10(OH)2)	7.8, 4.1[d]	none
Selenium	Se	79.0	8.52E-01	1.08E-05	CaSeO4	6.7E-05	none
Sodium	Na	23.0	2.14E+02	9.31E-03	Albite (NaAlSi3O8), Halite (NaCl), NaI, NaCN	14 (4), 9E-04, 9.49E-07, 2.16E-04	none
Sulfate	SO4	96.0	2.05E+01	2.14E-04	Gypsum (CaSO4.2H2O), Barite (BaSO4)	0.0036, 0.022	none
Sulfide	S	32.1	7.59E+02	2.36E-02	Pyrite (FeS2), Sphalerite (ZnS)	0.34, 0.053	oxidized to SO4
Technitium (rad)	Tc	98.9	3.40E-04	3.43E-09	TcO2.2H20(amorphous)	5.72E-08	none
Tellurium (rad)	Te	128.0	2.38E-11	1.86E-16	not considered[g]	not considered[g]	not considered[g]
Terbium	Tb	158.9	5.73E+02	3.61E-03	Tb2O3	3E-02	none
Uranium (rad)	U	238.0	5.94E+00	2.49E-05	CaUO4	4.16E-04	CaUO4
Vanadium	V	50.9	2.15E+01	4.22E-04	Ca2V2O7	3.5E-03	Ca2V2O7
Ytterbium	Yb	173.0	1.95E+02	1.13E-03	Yb2O3	9.4E-03	Yb(OH)3
Zinc	Zn	65.4	2.08E+02	3.18E-03	Sphalerite (ZnS)	5E-02	Zincite (ZnCO3)

Notes:

a. Radioactive constituents expressed as total mass of all reported isotopes

b. Calculated by dividing the kg of each constituent by 5.85E+08 kg, the total inventory mass.

c. Calculated by multiplying the moles/kg value by 16.7 (the number of kg soil exposed to 1L of leachate) and dividing by constituent's stochiometry in the mineral. Input into PHREEQC.

d. Moles of these minerals were derived from observed mineral abundance and not from design inventory (see text)

e. Radioactive carbon could not be considered separately from non-radioactive carbon, and was assumed to be completely soluble

f. Nitrite was not considered stable in soil, and was not considered in the analysis

g. No solubility data was found for tellurium, so it was assumed to be completely soluble

Table A-6. Organic Compounds from Design Inventory
Calculated mg/L assuming complete dissolution

constituent	tot kg	5.8504E+08 mg/kg	0.0638 * mg/L
1,1,1-Trichloroethane f	9.175492298	1.5684E-02	2.4583E-01
1,1,2,2-Tetrachloroethane	0.028938608	4.9465E-05	7.7531E-04
1,1,2-Trichloroethane	0.141619589	2.4207E-04	3.7942E-03
1,1-Dichloroethane	1.368989357	2.3400E-03	3.6677E-02
1,1-Dichloroethene	0.865453042	1.4793E-03	2.3187E-02
1,2,4-Trichlorobenzene	6.655879888	1.1377E-02	1.7832E-01
1,2-Dichlorobenzene	6.655879888	1.1377E-02	1.7832E-01
1,2-Dichloroethane	0.003147102	5.3793E-06	8.4316E-05
1,2-Dichloroethene (total)	0.189636546	3.2415E-04	5.0806E-03
1,3-Dichlorobenzene	6.655879888	1.1377E-02	1.7832E-01
1,4-Dichlorobenzene	263.2739454	4.5001E-01	7.0535E+00
1,4-Dioxane g	0.010999277	1.8801E-05	2.9469E-04
2,4,5-Trichlorophenol	26.0930445	4.4601E-02	6.9907E-01
2,4,6-Trichlorophenol	10.67926988	1.8254E-02	2.8611E-01
2,4-Dichlorophenol	12.63537363	2.1598E-02	3.3852E-01
2,4-Dimethylphenol	10.67926988	1.8254E-02	2.8611E-01
2,4-Dinitrophenol	29.79645552	5.0931E-02	7.9829E-01
2,4-Dinitrotoluene	6.655879888	1.1377E-02	1.7832E-01
2,6-Dinitrotoluene	12.09928988	2.0681E-02	3.2416E-01
2-Butanone	14.45966536	2.4716E-02	3.8740E-01
2-Chloronaphthalene	6.655879888	1.1377E-02	1.7832E-01
2-Chlorophenol	10.67926988	1.8254E-02	2.8611E-01
2-Hexanone	1.577610208	2.6966E-03	4.2267E-02
2-Methylnaphthalene	299.4425884	5.1184E-01	8.0225E+00
2-Methylphenol	12.07213869	2.0635E-02	3.2343E-01
2-Nitroaniline	15.91623451	2.7206E-02	4.2642E-01
2-Nitrophenol	10.67926988	1.8254E-02	2.8611E-01
3,3'-Dichlorobenzidine	6.655879888	1.1377E-02	1.7832E-01
3-Methyl Butanal g	0.130604732	2.2324E-04	3.4991E-03
3-Nitroaniline	15.91623451	2.7206E-02	4.2642E-01
4,6-Dinitro-2-methylphenol	26.0930445	4.4601E-02	6.9907E-01
4-Bromophenyl-phenylether	6.655879888	1.1377E-02	1.7832E-01
4-Chloro-3-methylphenol	10.67926988	1.8254E-02	2.8611E-01
4-Chloroaniline	23.86523056	4.0793E-02	6.3939E-01
4-Chlorophenyl-phenylether	6.655879888	1.1377E-02	1.7832E-01
4-Methyl-2-Pentanone f	17.33648341	2.9633E-02	4.6447E-01
4-Methylphenol	22.56936671	3.8578E-02	6.0467E-01
4-Nitroaniline	15.91623451	2.7206E-02	4.2642E-01
4-Nitrophenol	30.1607092	5.1554E-02	8.0805E-01
Acenaphthene	118.3160089	2.0224E-01	3.1699E+00
Acenaphthylene	12.09928988	2.0681E-02	3.2416E-01
Acetone f	362.9988875	6.2047E-01	9.7253E+00
Acetonitrile g	0.010999277	1.8801E-05	2.9469E-04
Acrolein g	0.005299652	9.0587E-06	1.4199E-04
Acrylonitrile g	0.005299652	9.0587E-06	1.4199E-04
Anthracene	187.3670094	3.2027E-01	5.0198E+00
Aramite g	0.066995597	1.1452E-04	1.7949E-03

Table A-6. Organic Compounds from Design Inventory
Calculated mg/L assuming complete dissolution

constituent	tot kg	5.8504E+08 mg/kg	0.0638 * mg/L
Aroclor-1016	4.496729992	7.6863E-03	1.2047E-01
Aroclor-1254	75.10023766	1.2837E-01	2.0120E+00
Aroclor-1260	421.5951954	7.2063E-01	1.1295E+01
Aroclor-1268	36.36971761	6.2167E-02	9.7440E-01
Benzene f	352.9562773	6.0331E-01	9.4562E+00
Benzidine g	0.169988829	2.9056E-04	4.5543E-03
Benzo(a)anthracene	148.0297692	2.5303E-01	3.9659E+00
Benzo(a)pyrene	61.33643527	1.0484E-01	1.6433E+00
Benzo(b)fluoranthene	104.9909475	1.7946E-01	2.8129E+00
Benzo(g,h,i)perylene	6.655879888	1.1377E-02	1.7832E-01
Benzo(k)fluoranthene	10.87999323	1.8597E-02	2.9149E-01
Benzoic acid g	5.006356559	8.5574E-03	1.3413E-01
bis(2-Chloroethoxy)methane	6.655879888	1.1377E-02	1.7832E-01
bis(2-Chloroethyl)ether	6.655879888	1.1377E-02	1.7832E-01
bis(2-Chloroisopropyl)ether	6.655879888	1.1377E-02	1.7832E-01
bis(2-Ethylhexyl)phthalate	86.07887249	1.4713E-01	2.3062E+00
Butane,1,1,3,4-Tetrachloro- g	4.615064992	7.8885E-03	1.2364E-01
Butylbenzylphthalate	39.72844873	6.7908E-02	1.0644E+00
Carbazole	18.92344171	3.2346E-02	5.0699E-01
Carbon Disulfide f	26.63560996	4.5528E-02	7.1361E-01
Chlorobenzene	3.844185056	6.5709E-03	1.0299E-01
Chloroethane	0.001764757	3.0165E-06	4.7280E-05
Chloromethane	0.206368875	3.5275E-04	5.5289E-03
Chrysene	155.1487311	2.6520E-01	4.1567E+00
Decane, 3,4-Dimethyl g	0.094413059	1.6138E-04	2.5295E-03
Diacetone alcohol g	2527.635596	4.3205E+00	6.7719E+01
Dibenz(a,h)anthracene	6.655879888	1.1377E-02	1.7832E-01
Dibenzofuran	189.6466875	3.2416E-01	5.0809E+00
Diethylphthalate	6.659079678	1.1382E-02	1.7841E-01
Dimethyl Disulfide g	1.730906083	2.9586E-03	4.6374E-02
Dimethylphthalate	6.655879888	1.1377E-02	1.7832E-01
Di-n-butylphthalate	13.95355046	2.3851E-02	3.7384E-01
Di-n-octylphthalate	15.33901522	2.6219E-02	4.1096E-01
Eicosane g	1.656689997	2.8318E-03	4.4385E-02
Ethyl cyanide g	0.010999277	1.8801E-05	2.9469E-04
Ethylbenzene	45.67776881	7.8077E-02	1.2238E+00
Famphur g	0.033997766	5.8112E-05	9.1085E-04
Fluoranthene	446.0559137	7.6244E-01	1.1951E+01
Fluorene	107.3916964	1.8356E-01	2.8772E+00
Heptadecane, 2,6,10,15-Tetra g	2.011694997	3.4386E-03	5.3896E-02
Hexachlorobenzene	6.655879888	1.1377E-02	1.7832E-01
Hexachlorobutadiene	12.09928988	2.0681E-02	3.2416E-01
Hexachlorocyclopentadiene	6.655879888	1.1377E-02	1.7832E-01
Hexachloroethane	6.655879888	1.1377E-02	1.7832E-01
Indeno(1,2,3-cd)pyrene	6.655879888	1.1377E-02	1.7832E-01
Isobutyl alcohol g	0.010999277	1.8801E-05	2.9469E-04
Isophorone	6.65827973	1.1381E-02	1.7839E-01

Table A-6. Organic Compounds from Design Inventory
Calculated mg/L assuming complete dissolution

constituent	tot kg	5.8504E+08 mg/kg	0.0638 * mg/L
Isopropyl Alcohol/2-propanol g	1.241278203	2.1217E-03	3.3256E-02
Kepone g	58.03510406	9.9199E-02	1.5548E+00
Mesityl oxide g	49.58236491	8.4751E-02	1.3284E+00
Methyl Acetate g	0.283239177	4.8414E-04	7.5884E-03
Methylene Chloride	48.91817499	8.3616E-02	1.3106E+00
Naphthalene	248.7161768	4.2513E-01	6.6635E+00
Nitrobenzene	6.655879888	1.1377E-02	1.7832E-01
N-Nitroso-di-n-propylamine	6.655879888	1.1377E-02	1.7832E-01
N-Nitrosodiphenylamine	6.655879888	1.1377E-02	1.7832E-01
Octane,2,3,7-Trimethyl g	0.094413059	1.6138E-04	2.5295E-03
o-Toluenesulfonamide g	2.958374995	5.0567E-03	7.9259E-02
Pentachlorophenol	32.69898432	5.5892E-02	8.7605E-01
Phenanthrene	683.4377181	1.1682E+00	1.8310E+01
Phenol	46.67445686	7.9781E-02	1.2505E+00
Phenol,2,6-Bis(1,1-Dimethyl) g	2.366699996	4.0454E-03	6.3407E-02
p-Toluenesulfonamide g	2.958374995	5.0567E-03	7.9259E-02
Pyrene	148.1681822	2.5326E-01	3.9696E+00
Styrene	0.000599961	1.0255E-06	1.6074E-05
Tetrachloroethene f	5.637621485	9.6364E-03	1.5104E-01
Toluene f	574.50195	9.8199E-01	1.5392E+01
Tributylphosphate	212.6773638	3.6353E-01	5.6979E+00
Trichloroethene f	42.14465605	7.2038E-02	1.1291E+00
Undecane,4,6-Dimethyl- g	0.094413059	1.6138E-04	2.5295E-03
Xylene (ortho) f	2.271559432	3.8828E-03	6.0858E-02
Xylene (total) f	2020.870091	3.4543E+00	5.4142E+01
		total mg/L=	2.9048E+02

* Assume H2O density = 1.064 (from PHREEQC) and mass moisture content = 6%)

Appendix B

PHREEQC Input and Output Files

Appendix B
PHREEQC Input File

```
TITLE Test Screened Constituents(assume 1L water, 16.7 kg soil), mix
rain and applied water, solubles as REACTION
SOLUTION 1 Average Rainfall Composition
        units   mg/L
        pH      5.6
        pe      8.451
        temp    25.0
        redox   O(0)/O(-2)
        O(0)            1.0     O2(g) -0.7
Na    2
K     0.27
Ca    0.13
Mg    0.27
C     0.36
Cl    3.8
S(6)  0.62
SOLUTION 2 INEEL Water Quality (CPP-1, 6/6/91)
units  mg/L
pH    8
pe     8.4
redox   O(0)/O(-2)
        O(0)            1.0     O2(g) -0.7
C     194
Ca    54
Mg    14
Na    7.9
K     2.5
Cl    18
S(6)  22
MIX 1 Mixing Solutions 1 and 2
1   0.85
2   0.15
SAVE SOLUTION  3
END
USE SOLUTION  3
REACTION
NaCN  2.16e-04
NaI   9.49e-07
1.0
EQUILIBRIUM_PHASES 1
Calcite     0.0  6.1
Illite      0.0   4.1
Kaolinite   0.0  0.0
Quartz      0.0  106.5
Gypsum      0.0   0.0013
Albite      0.0  14.4
```

```
K-Feldspar  0.0  7.8
Fluorapatite  0.0  0.017
Dolomite  0.0   Enstatite  21.7
Yb2O3  0.0  0.0094
Fe(OH)3  0.0  2.89
Pyrite  0.0  0.17
Zincite  0.0  Sphalerite  0.05
Birnessite  0.0  0.008
Barite  0.0  0.022
Borax  0.0  0.07
PuO2   0.0  8.76e-09
CaUO4  0.0  0.000417
Ca2V2O7  0.0  0.0035
Tb2O3    0.0  0.03
TcO2:2H2O(am)   0.0  5.72e-08
Ca3(AsO4)2  0.0  0.0006
Niter  0.0  0.001
Halite    0.0  0.0009
CaSeO4    0.0  1.8e-04
O2(g)   -0.7   1.0
CO2(g)    -3.5   1.0
END
```

B-2 PHREEQC Output File

```
Input file: C:\Documents\INEEL\pqe2\EDF274_update.pqi
  Output file: C:\Documents\INEEL\pqe2\EDF274_update.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive\llnl.dat

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

      LLNL_AQUEOUS_MODEL_PARAMETERS
      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\USGS\Phreeqc Interactive\llnl.dat
      TITLE Test new Screening Assemblage (assume 1kg water, 6.2 kg
soil), mix rain and applied water, solubles as PHASES
      SOLUTION 1 Average Rainfall Composition
              units   mg/L
              pH      5.6
              pe      8.451
              temp    25.0
              redox   O(0)/O(-2)
              O(0)            1.0     O2(g) -0.7
      Na    2
      K     0.27
      Ca    0.13
      Mg    0.27
      C     0.36
      Cl    3.8
      S(6)  0.62
      SOLUTION 2 INEEL Water Quality (CPP-1, 6/6/91)
      units  mg/L
      pH    8
      pe     8.4
      redox   O(0)/O(-2)
              O(0)            1.0     O2(g) -0.7
      C     194
      Ca    54
      Mg    14
```

```
     Na    7.9
     K     2.5
     Cl    18
     S(6)  22
     MIX 1 Mixing Solutions 1 and 2
     1   0.85
     2   0.15
     SAVE SOLUTION  3
     END
-----
TITLE
-----

 Test new Screening Assemblage (assume 1kg water, 6.2 kg soil), mix
rain and applied water, solubles as PHASES

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

Initial solution 1.   Average Rainfall Composition

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

     Elements           Molality       Moles

     C                5.902e-006  5.902e-006
     Ca               3.244e-006  3.244e-006
     Cl               1.072e-004  1.072e-004
     K                6.906e-006  6.906e-006
     Mg               1.111e-005  1.111e-005
     Na               8.700e-005  8.700e-005
     O(0)             5.113e-004  5.113e-004  Equilibrium with
O2(g)
     S(6)             6.456e-006  6.456e-006

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

                                        pH  =   5.600
                                        pe  =   8.451
                          Activity of water  =   1.000
                             Ionic strength  =  1.438e-004
                         Mass of water (kg)  =  1.000e+000
                   Total alkalinity (eq/kg)  = -1.669e-006
                         Total CO2 (mol/kg)  =  5.902e-006
                       Temperature (deg C)   =  25.000
                    Electrical balance (eq)  =  4.179e-006
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =   1.70
                                Iterations  =   4
                                   Total H  = 1.110507e+002
```

Total O = 5.552587e+001

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	15.0007	0.8874

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.546e-006	2.512e-006	-5.594	-5.600	-0.006
OH-	3.889e-009	3.836e-009	-8.410	-8.416	-0.006
H2O	5.553e+001	1.000e+000	-0.000	-0.000	0.000
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-266.969	-266.969	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-239.283	-239.283	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-148.571	-148.571	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-51.542	-51.542	0.000
C(4)	5.902e-006				
CO2	5.027e-006	5.027e-006	-5.299	-5.299	0.000
HCO3-	8.748e-007	8.627e-007	-6.058	-6.064	-0.006
MgHCO3+	1.067e-010	1.052e-010	-9.972	-9.978	-0.006
NaHCO3	1.059e-010	1.059e-010	-9.975	-9.975	0.000
CaHCO3+	3.179e-011	3.136e-011	-10.498	-10.504	-0.006
CO3-2	1.611e-011	1.524e-011	-10.793	-10.817	-0.024
MgCO3	1.692e-013	1.692e-013	-12.771	-12.771	0.000
CaCO3	1.083e-013	1.083e-013	-12.965	-12.965	0.000

```
     NaCO3-          4.638e-015  4.574e-015   -14.334   -14.340
-0.006
Ca              3.244e-006
     Ca+2            3.241e-006  3.067e-006    -5.489    -5.513
-0.024
     CaSO4           2.725e-009  2.725e-009    -8.565    -8.565
0.000
     CaCl+           6.967e-011  6.871e-011   -10.157   -10.163
-0.006
     CaHCO3+         3.179e-011  3.136e-011   -10.498   -10.504
-0.006
     CaOH+           1.749e-013  1.725e-013   -12.757   -12.763
-0.006
     CaCO3           1.083e-013  1.083e-013   -12.965   -12.965
0.000
     CaCl2           8.542e-015  8.542e-015   -14.068   -14.068
0.000
Cl(-1)          1.072e-004
     Cl-             1.072e-004  1.057e-004    -3.970    -3.976
-0.006
     NaCl            1.594e-009  1.594e-009    -8.798    -8.798
0.000
     MgCl+           8.786e-010  8.665e-010    -9.056    -9.062
-0.006
     CaCl+           6.967e-011  6.871e-011   -10.157   -10.163
-0.006
     HCl             5.963e-011  5.963e-011   -10.225   -10.225
0.000
     KCl             2.417e-011  2.417e-011   -10.617   -10.617
0.000
     CaCl2           8.542e-015  8.542e-015   -14.068   -14.068
0.000
Cl(1)           1.233e-019
     HClO            1.219e-019  1.219e-019   -18.914   -18.914
0.000
     ClO-            1.327e-021  1.309e-021   -20.877   -20.883
-0.006
Cl(3)           2.103e-031
     ClO2-           2.095e-031  2.066e-031   -30.679   -30.685
-0.006
     HClO2           7.674e-034  7.674e-034   -33.115   -33.115
0.000
Cl(5)           2.354e-027
     ClO3-           2.354e-027  2.321e-027   -26.628   -26.634
-0.006
Cl(7)           1.320e-027
     ClO4-           1.320e-027  1.301e-027   -26.880   -26.886
-0.006
H(0)            0.000e+000
     H2              0.000e+000  0.000e+000   -44.302   -44.302
0.000
K               6.906e-006
```

```
     K+                  6.905e-006  6.810e-006    -5.161    -5.167
-0.006
     KSO4-               3.390e-010  3.343e-010    -9.470    -9.476
-0.006
     KCl                 2.417e-011  2.417e-011   -10.617   -10.617
0.000
     KOH                 9.400e-015  9.400e-015   -14.027   -14.027
0.000
     KHSO4               7.410e-016  7.410e-016   -15.130   -15.130
0.000
Mg                 1.111e-005
     Mg+2                1.109e-005  1.050e-005    -4.955    -4.979
-0.024
     MgSO4               1.706e-008  1.706e-008    -7.768    -7.768
0.000
     MgCl+               8.786e-010  8.665e-010    -9.056    -9.062
-0.006
     MgHCO3+             1.067e-010  1.052e-010    -9.972    -9.978
-0.006
     MgCO3               1.692e-013  1.692e-013   -12.771   -12.771
0.000
     Mg4(OH)4+4          6.773e-038  5.429e-038   -37.169   -37.265
-0.096
Na                 8.700e-005
     Na+                 8.699e-005  8.579e-005    -4.061    -4.067
-0.006
     NaSO4-              3.496e-009  3.448e-009    -8.456    -8.462
-0.006
     NaCl                1.594e-009  1.594e-009    -8.798    -8.798
0.000
     NaHCO3              1.059e-010  1.059e-010    -9.975    -9.975
0.000
     NaOH                5.677e-014  5.677e-014   -13.246   -13.246
0.000
     NaCO3-              4.638e-015  4.574e-015   -14.334   -14.340
-0.006
O(0)               5.113e-004
     O2                  2.556e-004  2.556e-004    -3.592    -3.592
0.000
S(6)               6.456e-006
     SO4-2               6.430e-006  6.083e-006    -5.192    -5.216
-0.024
     MgSO4               1.706e-008  1.706e-008    -7.768    -7.768
0.000
     NaSO4-              3.496e-009  3.448e-009    -8.456    -8.462
-0.006
     CaSO4               2.725e-009  2.725e-009    -8.565    -8.565
0.000
     HSO4-               1.565e-009  1.543e-009    -8.805    -8.812
-0.006
     KSO4-               3.390e-010  3.343e-010    -9.470    -9.476
-0.006
```

```
     KHSO4              7.410e-016  7.410e-016   -15.130   -15.130
0.000
     H2SO4              3.658e-018  3.658e-018   -17.437   -17.437
0.000

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

     Phase                SI log IAP  log KT

     Anhydrite          -6.38  -10.73   -4.35  CaSO4
     Antarcticite      -17.56  -13.47    4.09  CaCl2:6H2O
     Aphthitalite      -26.11  -30.00   -3.89  NaK3(SO4)2
     Aragonite          -7.95   -5.98    1.97  CaCO3
     Arcanite          -13.71  -15.55   -1.84  K2SO4
     Artinite          -18.85    0.78   19.63  Mg2CO3(OH)2:3H2O
     Bassanite          -7.02  -10.73   -3.71  CaSO4:0.5H2O
     Bischofite        -17.32  -12.93    4.39  MgCl2:6H2O
     Bloedite          -21.07  -23.54   -2.48  Na2Mg(SO4)2:4H2O
     Brucite           -10.06    6.22   16.28  Mg(OH)2
     Burkeite          -44.78  -35.30    9.49  Na6CO3(SO4)2
     C                 -72.22   -8.07   64.15  C
     C(g)             -189.84   -8.07  181.77  C
     Ca               -132.35    7.48  139.83  Ca
     Ca(g)            -157.59    7.48  165.07  Ca
     Ca2Cl2(OH)2:H2O -34.07   -7.78   26.29  Ca2Cl2(OH)2:H2O
     Ca4Cl2(OH)6:13H2O -64.73    3.59   68.33  Ca4Cl2(OH)6:13H2O
     Calcite            -7.80   -5.98    1.82  CaCO3
     Carnallite        -26.35  -22.07    4.27  KMgCl3:6H2O
     CaSO4:0.5H2O(beta)  -7.19  -10.73   -3.54  CaSO4:0.5H2O
     CH4(g)           -145.73   -4.48  141.25  CH4
     Chloromagnesite -34.75  -12.93   21.82  MgCl2
     Cl2(g)            -23.94  -20.95    2.99  Cl2
     CO(g)             -48.54   -9.87   38.68  CO
     CO2(g)             -3.84  -11.66   -7.83  CO2
     Dolomite          -13.89  -11.42    2.47  CaMg(CO3)2
     Dolomite-dis      -15.43  -11.42    4.01  CaMg(CO3)2
     Dolomite-ord      -13.88  -11.42    2.46  CaMg(CO3)2
     Epsomite           -8.23  -10.19   -1.96  MgSO4:7H2O
     Gaylussite        -25.74  -14.57   11.16  CaNa2(CO3)2:5H2O
     Glauberite        -18.61  -24.08   -5.47  Na2Ca(SO4)2
     Gypsum             -6.20  -10.73   -4.53  CaSO4:2H2O
     H2(g)             -41.20    1.80   43.00  H2
     H2O(g)             -1.59   -0.00    1.59  H2O
     Halite             -9.61   -8.04    1.56  NaCl
     HCl(g)            -15.88   -9.58    6.30  HCl
     Hexahydrite        -8.47  -10.19   -1.73  MgSO4:6H2O
     Huntite           -32.52  -22.31   10.22  CaMg3(CO3)4
     Hydromagnesite    -46.29  -15.55   30.74  Mg5(CO3)4(OH)2:4H2O
     Hydrophilite      -25.21  -13.47   11.75  CaCl2
     Ice                -0.14   -0.00    0.14  H2O
     K                 -69.65    1.33   70.98  K
```

K(g)	-80.25	1.33	81.58	K
K2CO3:1.5H2O	-24.18	-10.80	13.38	K2CO3:1.5H2O
K2O	-83.17	0.87	84.04	K2O
K3H(SO4)2	-27.91	-31.53	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-94.23	-66.52	27.71	K8H4(CO3)6:3H2O
Kainite	-19.03	-19.34	-0.31	KMgClSO4:3H2O
Kalicinite	-11.51	-11.23	0.28	KHCO3
Kieserite	-9.93	-10.19	-0.27	MgSO4:H2O
KMgCl3	-43.32	-22.07	21.25	KMgCl3
KMgCl3:2H2O	-36.04	-22.07	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-19.96	-9.70	10.26	KNaCO3:6H2O
Lansfordite	-10.28	-5.44	4.84	MgCO3:5H2O
Leonite	-21.63	-25.74	-4.11	K2Mg(SO4)2:4H2O
Lime	-26.88	5.69	32.57	CaO
Magnesite	-7.72	-5.44	2.27	MgCO3
Mercallite	-14.54	-15.98	-1.44	KHSO4
Mg	-114.50	8.02	122.52	Mg
Mg(g)	-134.23	8.02	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-13.83	-8.64	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-16.29	-7.08	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-25.66	-12.93	12.73	MgCl2:2H2O
MgCl2:4H2O	-20.23	-12.93	7.30	MgCl2:4H2O
MgCl2:H2O	-29.00	-12.93	16.07	MgCl2:H2O
MgOHCl	-19.25	-3.35	15.89	MgOHCl
MgSO4	-15.02	-10.19	4.83	MgSO4
Mirabilite	-12.19	-13.35	-1.15	Na2SO4:10H2O
Misenite	-100.37	-111.45	-11.08	K8H6(SO4)7
Monohydrocalcite	-8.66	-5.98	2.68	CaCO3:H2O
Na	-64.94	2.43	67.37	Na
Na(g)	-78.43	2.43	80.86	Na
Na2CO3	-19.76	-8.60	11.16	Na2CO3
Na2CO3:7H2O	-18.54	-8.60	9.94	Na2CO3:7H2O
Na2O	-64.35	3.07	67.42	Na2O
Na3H(SO4)2	-27.34	-28.23	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-31.53	-37.43	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-9.99	-10.13	-0.14	NaHCO3
Natron	-18.19	-8.60	9.59	Na2CO3:10H2O
Nesquehonite	-10.73	-5.44	5.29	MgCO3:3H2O
O2(g)	-0.70	-3.59	-2.89	O2
Oxychloride-Mg	-22.97	2.87	25.83	Mg2Cl(OH)3:4H2O
Pentahydrite	-8.81	-10.19	-1.39	MgSO4:5H2O
Periclase	-15.10	6.22	21.33	MgO
Picromerite	-21.30	-25.74	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-25.90	-14.57	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-32.89	-47.20	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-16.86	5.69	22.55	Ca(OH)2
Starkeyite	-9.19	-10.19	-1.00	MgSO4:4H2O
Sylvite	-9.97	-9.14	0.83	KCl
Syngenite	-18.68	-26.28	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-56.47	-39.33	17.14	Mg2CaCl6:12H2O
Thenardite	-12.99	-13.35	-0.36	Na2SO4

```
     Thermonatrite    -19.53   -8.60   10.94  Na2CO3:H2O
     Trona-K          -32.52  -20.93   11.59  K2NaH(CO3)2:2H2O

Initial solution 2.   INEEL Water Quality (CPP-1, 6/6/91)

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

     Elements            Molality       Moles

     C                 3.181e-003  3.181e-003
     Ca                1.348e-003  1.348e-003
     Cl                5.079e-004  5.079e-004
     K                 6.396e-005  6.396e-005
     Mg                5.762e-004  5.762e-004
     Na                3.437e-004  3.437e-004
     O(0)              5.105e-004  5.105e-004  Equilibrium with
O2(g)
     S(6)              2.291e-004  2.291e-004

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

                                        pH  =   8.000
                                        pe  =   8.400
                          Activity of water  =   1.000
                             Ionic strength  =  6.037e-003
                        Mass of water (kg)   =  1.000e+000
                  Total alkalinity (eq/kg)   =  3.167e-003
                        Total CO2 (mol/kg)   =  3.181e-003
                      Temperature (deg C)    =  25.000
                   Electrical balance (eq)   =  1.228e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =   1.53
                                Iterations  =   5
                                   Total H  = 1.110537e+002
                                   Total O  = 5.553623e+001

---------------------------------Redox couples----------------------
-----------

     Redox couple              pe  Eh (volts)

     O(-2)/O(0)          12.6007      0.7454

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

                                                   Log       Log
Log
     Species             Molality    Activity  Molality  Activity
Gamma
```

```
     OH-                1.047e-006  9.634e-007    -5.980    -6.016
-0.036
     H+                 1.077e-008  1.000e-008    -7.968    -8.000
-0.032
     H2O                5.553e+001  9.999e-001    -0.000    -0.000
0.000
C(-2)             0.000e+000
     C2H4               0.000e+000  0.000e+000  -264.752  -264.752
0.000
C(-3)             0.000e+000
     C2H6               0.000e+000  0.000e+000  -237.066  -237.066
0.000
C(-4)             0.000e+000
     CH4                0.000e+000  0.000e+000  -147.463  -147.463
0.000
C(2)              0.000e+000
     CO                 0.000e+000  0.000e+000   -50.433   -50.433
0.000
C(4)              3.181e-003
     HCO3-              3.020e-003  2.781e-003    -2.520    -2.556
-0.036
     CO2                6.441e-005  6.451e-005    -4.191    -4.190
0.001
     CaHCO3+            3.309e-005  3.047e-005    -4.480    -4.516
-0.036
     CaCO3              2.644e-005  2.644e-005    -4.578    -4.578
0.000
     CO3-2              1.712e-005  1.234e-005    -4.766    -4.909
-0.142
     MgHCO3+            1.403e-005  1.292e-005    -4.853    -4.889
-0.036
     MgCO3              5.221e-006  5.221e-006    -5.282    -5.282
0.000
     NaHCO3             1.253e-006  1.253e-006    -5.902    -5.902
0.000
     NaCO3-             1.477e-008  1.360e-008    -7.831    -7.866
-0.036
Ca                1.348e-003
     Ca+2               1.269e-003  9.247e-004    -2.896    -3.034
-0.138
     CaHCO3+            3.309e-005  3.047e-005    -4.480    -4.516
-0.036
     CaCO3              2.644e-005  2.644e-005    -4.578    -4.578
0.000
     CaSO4              1.890e-005  1.890e-005    -4.724    -4.724
0.000
     CaCl+              9.928e-008  9.143e-008    -7.003    -7.039
-0.036
     CaOH+              1.418e-008  1.306e-008    -7.848    -7.884
-0.036
     CaCl2              5.017e-011  5.017e-011   -10.300   -10.300
0.000
```

```
Cl(-1)          5.079e-004
     Cl-              5.076e-004  4.665e-004    -3.294    -3.331
-0.037
     MgCl+            1.582e-007  1.457e-007    -6.801    -6.837
-0.036
     CaCl+            9.928e-008  9.143e-008    -7.003    -7.039
-0.036
     NaCl             2.583e-008  2.583e-008    -7.588    -7.588
0.000
     KCl              9.198e-010  9.198e-010    -9.036    -9.036
0.000
     CaCl2            5.017e-011  5.017e-011   -10.300   -10.300
0.000
     HCl              1.048e-012  1.048e-012   -11.980   -11.980
0.000
Cl(1)           8.416e-021
     ClO-             6.274e-021  5.777e-021   -20.202   -20.238
-0.036
     HClO             2.143e-021  2.143e-021   -20.669   -20.669
0.000
Cl(3)           9.904e-031
     ClO2-            9.904e-031  9.120e-031   -30.004   -30.040
-0.036
     HClO2            1.348e-035  1.348e-035   -34.870   -34.870
0.000
Cl(5)           1.114e-026
     ClO3-            1.114e-026  1.024e-026   -25.953   -25.990
-0.036
Cl(7)           6.244e-027
     ClO4-            6.244e-027  5.744e-027   -26.205   -26.241
-0.036
H(0)            0.000e+000
     H2               0.000e+000  0.000e+000   -44.302   -44.302
0.001
K               6.396e-005
     K+               6.389e-005  5.872e-005    -4.195    -4.231
-0.037
     KSO4-            7.201e-008  6.631e-008    -7.143    -7.178
-0.036
     KCl              9.198e-010  9.198e-010    -9.036    -9.036
0.000
     KOH              2.036e-011  2.036e-011   -10.691   -10.691
0.000
     KHSO4            5.851e-016  5.851e-016   -15.233   -15.233
0.000
Mg              5.762e-004
     Mg+2             5.418e-004  4.001e-004    -3.266    -3.398
-0.132
     MgSO4            1.495e-005  1.495e-005    -4.825    -4.825
0.000
     MgHCO3+          1.403e-005  1.292e-005    -4.853    -4.889
-0.036
```

```
     MgCO3              5.221e-006  5.221e-006    -5.282    -5.282
0.000
     MgCl+              1.582e-007  1.457e-007    -6.801    -6.837
-0.036
     Mg4(OH)4+4         1.643e-021  4.554e-022   -20.784   -21.342
-0.557
Na               3.437e-004
     Na+                3.421e-004  3.151e-004    -3.466    -3.502
-0.036
     NaHCO3             1.253e-006  1.253e-006    -5.902    -5.902
0.000
     NaSO4-             3.163e-007  2.912e-007    -6.500    -6.536
-0.036
     NaCl               2.583e-008  2.583e-008    -7.588    -7.588
0.000
     NaCO3-             1.477e-008  1.360e-008    -7.831    -7.866
-0.036
     NaOH               5.236e-011  5.236e-011   -10.281   -10.281
0.000
O(0)             5.105e-004
     O2                 2.553e-004  2.556e-004    -3.593    -3.592
0.001
S(6)             2.291e-004
     SO4-2              1.949e-004  1.399e-004    -3.710    -3.854
-0.144
     CaSO4              1.890e-005  1.890e-005    -4.724    -4.724
0.000
     MgSO4              1.495e-005  1.495e-005    -4.825    -4.825
0.000
     NaSO4-             3.163e-007  2.912e-007    -6.500    -6.536
-0.036
     KSO4-              7.201e-008  6.631e-008    -7.143    -7.178
-0.036
     HSO4-              1.535e-010  1.413e-010    -9.814    -9.850
-0.036
     KHSO4              5.851e-016  5.851e-016   -15.233   -15.233
0.000
     H2SO4              1.333e-021  1.333e-021   -20.875   -20.875
0.000

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

     Phase               SI log IAP  log KT

     Anhydrite        -2.54   -6.89   -4.35  CaSO4
     Antarcticite    -13.79   -9.70    4.09  CaCl2:6H2O
     Aphthitalite    -20.02  -23.90   -3.89  NaK3(SO4)2
     Aragonite         0.44    2.41    1.97  CaCO3
     Arcanite        -10.47  -12.32   -1.84  K2SO4
     Artinite         -4.98   14.65   19.63  Mg2CO3(OH)2:3H2O
     Bassanite        -3.18   -6.89   -3.71  CaSO4:0.5H2O
```

Bischofite	-14.45	-10.06	4.39	MgCl2:6H2O
Bloedite	-15.63	-18.11	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-3.68	12.60	16.28	Mg(OH)2
Burkeite	-32.76	-23.27	9.49	Na6CO3(SO4)2
C	-71.11	-6.96	64.15	C
C(g)	-188.73	-6.96	181.77	C
Ca	-125.07	14.76	139.83	Ca
Ca(g)	-150.31	14.76	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.02	3.27	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-39.13	29.20	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.59	2.41	1.82	CaCO3
Carnallite	-21.89	-17.62	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-3.35	-6.89	-3.54	CaSO4:0.5H2O
CH4(g)	-144.62	-3.37	141.25	CH4
Chloromagnesite	-31.88	-10.06	21.82	MgCl2
Cl2(g)	-27.45	-24.46	2.99	Cl2
CO(g)	-47.44	-8.76	38.68	CO
CO2(g)	-2.73	-10.56	-7.83	CO2
Dolomite	1.98	4.46	2.47	CaMg(CO3)2
Dolomite-dis	0.44	4.46	4.01	CaMg(CO3)2
Dolomite-ord	1.99	4.46	2.46	CaMg(CO3)2
Epsomite	-5.29	-7.25	-1.96	MgSO4:7H2O
Gaylussite	-10.31	0.85	11.16	CaNa2(CO3)2:5H2O
Glauberite	-12.28	-17.75	-5.47	Na2Ca(SO4)2
Gypsum	-2.36	-6.89	-4.53	CaSO4:2H2O
H2(g)	-41.20	1.80	43.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-8.40	-6.83	1.56	NaCl
HCl(g)	-17.63	-11.33	6.30	HCl
Hexahydrite	-5.53	-7.25	-1.73	MgSO4:6H2O
Huntite	-1.67	8.55	10.22	CaMg3(CO3)4
Hydromagnesite	-9.95	20.79	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.44	-9.70	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-66.31	4.67	70.98	K
K(g)	-76.91	4.67	81.58	K
K2CO3:1.5H2O	-16.40	-3.02	13.38	K2CO3:1.5H2O
K2O	-76.50	7.54	84.04	K2O
K3H(SO4)2	-24.78	-28.40	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-60.89	-33.19	27.71	K8H4(CO3)6:3H2O
Kainite	-14.50	-14.81	-0.31	KMgClSO4:3H2O
Kalicinite	-7.07	-6.79	0.28	KHCO3
Kieserite	-6.99	-7.25	-0.27	MgSO4:H2O
KMgCl3	-38.87	-17.62	21.25	KMgCl3
KMgCl3:2H2O	-31.58	-17.62	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-12.55	-2.29	10.26	KNaCO3:6H2O
Lansfordite	-2.79	2.05	4.84	MgCO3:5H2O
Leonite	-15.46	-19.57	-4.11	K2Mg(SO4)2:4H2O
Lime	-19.60	12.97	32.57	CaO
Magnesite	-0.23	2.05	2.27	MgCO3
Mercallite	-14.65	-16.09	-1.44	KHSO4
Mg	-108.12	14.40	122.52	Mg

```
     Mg(g)              -127.85   14.40  142.25  Mg
     Mg1.25SO4(OH)0.5:0.5H2O  -9.30   -4.10    5.20
Mg1.25SO4(OH)0.5:0.5H2O
     Mg1.5SO4(OH)       -10.16   -0.95    9.21  Mg1.5SO4(OH)
     MgCl2:2H2O         -22.79  -10.06   12.73  MgCl2:2H2O
     MgCl2:4H2O         -17.36  -10.06    7.30  MgCl2:4H2O
     MgCl2:H2O          -26.13  -10.06   16.07  MgCl2:H2O
     MgOHCl             -14.62    1.27   15.89  MgOHCl
     MgSO4              -12.08   -7.25    4.83  MgSO4
     Mirabilite          -9.70  -10.86   -1.15  Na2SO4:10H2O
     Misenite           -97.75 -108.83  -11.08  K8H6(SO4)7
     Monohydrocalcite  -0.27    2.41    2.68  CaCO3:H2O
     Na                 -61.97    5.40   67.37  Na
     Na(g)              -75.46    5.40   80.86  Na
     Na2CO3             -12.72   -1.56   11.16  Na2CO3
     Na2CO3:7H2O        -11.50   -1.56    9.94  Na2CO3:7H2O
     Na2O               -58.42    9.00   67.42  Na2O
     Na3H(SO4)2         -25.32  -26.21   -0.89  Na3H(SO4)2
     Na4Ca(SO4)3:2H2O -22.71  -28.60   -5.89  Na4Ca(SO4)3:2H2O
     Nahcolite           -5.92   -6.06   -0.14  NaHCO3
     Natron             -11.15   -1.56    9.59  Na2CO3:10H2O
     Nesquehonite        -3.24    2.05    5.29  MgCO3:3H2O
     O2(g)               -0.70   -3.59   -2.89  O2
     Oxychloride-Mg     -11.96   13.87   25.83  Mg2Cl(OH)3:4H2O
     Pentahydrite        -5.87   -7.25   -1.39  MgSO4:5H2O
     Periclase           -8.72   12.60   21.33  MgO
     Picromerite        -15.13  -19.57   -4.44  K2Mg(SO4)2:6H2O
     Pirssonite         -10.47    0.85   11.32  Na2Ca(CO3)2:2H2O
     Polyhalite         -19.03  -33.35  -14.31  K2MgCa2(SO4)4:2H2O
     Portlandite         -9.58   12.97   22.55  Ca(OH)2
     Starkeyite          -6.25   -7.25   -1.00  MgSO4:4H2O
     Sylvite             -8.39   -7.56    0.83  KCl
     Syngenite          -11.60  -19.20   -7.60  K2Ca(SO4)2:H2O
     Tachyhydrite       -46.96  -29.82   17.14  Mg2CaCl6:12H2O
     Thenardite         -10.50  -10.86   -0.36  Na2SO4
     Thermonatrite      -12.50   -1.56   10.94  Na2CO3:H2O
     Trona-K            -20.66   -9.08   11.59  K2NaH(CO3)2:2H2O

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

Reaction step 1.

Using mix 1.     Mixing Solutions 1 and 2

Mixture 1. Mixing Solutions 1 and 2

       8.500e-001 Solution 1      Average Rainfall Composition
       1.500e-001 Solution 2      INEEL Water Quality (CPP-1, 6/6/91)
```

```
-----------------------------Solution composition-------------------
-----------

     Elements            Molality       Moles

     C                 4.822e-004  4.822e-004
     Ca                2.049e-004  2.049e-004
     Cl                1.673e-004  1.673e-004
     K                 1.546e-005  1.546e-005
     Mg                9.587e-005  9.587e-005
     Na                1.255e-004  1.255e-004
     S                 3.986e-005  3.986e-005

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

                                        pH  =   7.929      Charge
balance
                                        pe  =  12.671      Adjusted
to redox equilibrium
                        Activity of water  =   1.000
                           Ionic strength  =  1.062e-003
                       Mass of water (kg)  =  1.000e+000
                  Total alkalinity (eq/kg) =  4.736e-004
                       Total CO2 (mol/kg)  =  4.822e-004
                     Temperature (deg C)   =  25.000
                  Electrical balance (eq)  =  2.197e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   1.51
                               Iterations  =  14
                                  Total H  = 1.110511e+002
                                  Total O  = 5.552743e+001

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

                                                   Log       Log
Log
     Species             Molality    Activity  Molality  Activity
Gamma

     OH-               8.493e-007  8.185e-007    -6.071    -6.087
-0.016
     H+                1.219e-008  1.177e-008    -7.914    -7.929
-0.015
     H2O               5.553e+001  1.000e+000    -0.000    -0.000
0.000
C(-2)            0.000e+000
     C2H4              0.000e+000  0.000e+000  -266.194  -266.194
0.000
C(-3)            0.000e+000
     C2H6              0.000e+000  0.000e+000  -238.509  -238.509
0.000
```

```
C(-4)            0.000e+000
     CH4                 0.000e+000  0.000e+000  -148.184  -148.184
0.000
C(2)             0.000e+000
     CO                  0.000e+000  0.000e+000   -51.155   -51.155
0.000
C(4)             4.822e-004
     HCO3-               4.657e-004  4.489e-004    -3.332    -3.348
-0.016
     CO2                 1.225e-005  1.226e-005    -4.912    -4.912
0.000
     CO3-2               1.959e-006  1.692e-006    -5.708    -5.772
-0.064
     CaHCO3+             9.671e-007  9.322e-007    -6.015    -6.030
-0.016
     CaCO3               6.872e-007  6.872e-007    -6.163    -6.163
0.000
     MgHCO3+             4.440e-007  4.280e-007    -6.353    -6.369
-0.016
     MgCO3               1.469e-007  1.469e-007    -6.833    -6.833
0.000
     NaHCO3              7.761e-008  7.761e-008    -7.110    -7.110
0.000
     NaCO3-              7.423e-010  7.156e-010    -9.129    -9.145
-0.016
Ca               2.049e-004
     Ca+2                2.024e-004  1.752e-004    -3.694    -3.756
-0.063
     CaHCO3+             9.671e-007  9.322e-007    -6.015    -6.030
-0.016
     CaSO4               8.454e-007  8.454e-007    -6.073    -6.073
0.000
     CaCO3               6.872e-007  6.872e-007    -6.163    -6.163
0.000
     CaCl+               6.211e-009  5.987e-009    -8.207    -8.223
-0.016
     CaOH+               2.182e-009  2.103e-009    -8.661    -8.677
-0.016
     CaCl2               1.135e-012  1.135e-012   -11.945   -11.945
0.000
Cl(-1)           1.673e-004
     Cl-                 1.673e-004  1.612e-004    -3.777    -3.793
-0.016
     MgCl+               1.072e-008  1.033e-008    -7.970    -7.986
-0.016
     CaCl+               6.211e-009  5.987e-009    -8.207    -8.223
-0.016
     NaCl                3.424e-009  3.424e-009    -8.465    -8.465
0.000
     KCl                 8.063e-011  8.063e-011   -10.093   -10.093
0.000
```

```
     CaCl2              1.135e-012  1.135e-012   -11.945   -11.945
0.000
     HCl                4.261e-013  4.261e-013   -12.370   -12.370
0.000
Cl(1)             2.942e-021
     ClO-               2.071e-021  1.996e-021   -20.684   -20.700
-0.016
     HClO               8.713e-022  8.713e-022   -21.060   -21.060
0.000
Cl(3)             3.269e-031
     ClO2-              3.269e-031  3.151e-031   -30.486   -30.502
-0.016
     HClO2              5.483e-036  5.483e-036   -35.261   -35.261
0.000
Cl(5)             3.673e-027
     ClO3-              3.673e-027  3.540e-027   -26.435   -26.451
-0.016
Cl(7)             2.059e-027
     ClO4-              2.059e-027  1.985e-027   -26.686   -26.702
-0.016
H(0)              0.000e+000
     H2                 0.000e+000  0.000e+000   -44.302   -44.302
0.000
K                 1.546e-005
     K+                 1.546e-005  1.490e-005    -4.811    -4.827
-0.016
     KSO4-              4.119e-009  3.971e-009    -8.385    -8.401
-0.016
     KCl                8.063e-011  8.063e-011   -10.093   -10.093
0.000
     KOH                4.388e-012  4.388e-012   -11.358   -11.358
0.000
     KHSO4              4.124e-017  4.124e-017   -16.385   -16.385
0.000
Mg                9.587e-005
     Mg+2               9.455e-005  8.209e-005    -4.024    -4.086
-0.061
     MgSO4              7.239e-007  7.239e-007    -6.140    -6.140
0.000
     MgHCO3+            4.440e-007  4.280e-007    -6.353    -6.369
-0.016
     MgCO3              1.469e-007  1.469e-007    -6.833    -6.833
0.000
     MgCl+              1.072e-008  1.033e-008    -7.970    -7.986
-0.016
     Mg4(OH)4+4         7.510e-025  4.206e-025   -24.124   -24.376
-0.252
Na                1.255e-004
     Na+                1.254e-004  1.209e-004    -3.902    -3.918
-0.016
     NaHCO3             7.761e-008  7.761e-008    -7.110    -7.110
0.000
```

```
     NaSO4-            2.736e-008  2.637e-008    -7.563    -7.579
-0.016
     NaCl              3.424e-009  3.424e-009    -8.465    -8.465
0.000
     NaCO3-            7.423e-010  7.156e-010    -9.129    -9.145
-0.016
     NaOH              1.707e-011  1.707e-011   -10.768   -10.768
0.000
O(0)             5.112e-004
     O2                2.556e-004  2.556e-004    -3.592    -3.592
0.000
     S3O6-2            0.000e+000  0.000e+000  -183.903  -183.967
-0.064
     S2-2              0.000e+000  0.000e+000  -255.491  -255.555
-0.064
     S4O6-2            0.000e+000  0.000e+000  -277.572  -277.636
-0.064
     S3-2              0.000e+000  0.000e+000  -362.583  -362.646
-0.064
     S5O6-2            0.000e+000  0.000e+000  -400.120  -400.184
-0.064
     S4-2              0.000e+000  0.000e+000  -469.901  -469.965
-0.064
     S5-2              0.000e+000  0.000e+000  -577.436  -577.500
-0.064
S(-2)            0.000e+000
     HS-               0.000e+000  0.000e+000  -143.492  -143.508
-0.016
     H2S               0.000e+000  0.000e+000  -144.428  -144.428
0.000
     S-2               0.000e+000  0.000e+000  -148.442  -148.505
-0.063
     S2-2              0.000e+000  0.000e+000  -255.491  -255.555
-0.064
     S3-2              0.000e+000  0.000e+000  -362.583  -362.646
-0.064
     S4-2              0.000e+000  0.000e+000  -469.901  -469.965
-0.064
     S5-2              0.000e+000  0.000e+000  -577.436  -577.500
-0.064
S(2)             0.000e+000
     S2O3-2            0.000e+000  0.000e+000  -151.046  -151.110
-0.064
     HS2O3-            0.000e+000  0.000e+000  -158.009  -158.025
-0.016
S(3)             0.000e+000
     S2O4-2            0.000e+000  0.000e+000  -140.267  -140.331
-0.063
S(4)             0.000e+000
     SO3-2             0.000e+000  0.000e+000   -49.239   -49.303
-0.064
```

```
     HSO3-              0.000e+000  0.000e+000   -49.985   -50.000
-0.016
     H2SO3              0.000e+000  0.000e+000   -55.948   -55.948
0.000
     SO2                0.000e+000  0.000e+000   -56.048   -56.048
0.000
     S2O5-2             0.000e+000  0.000e+000  -104.767  -104.831
-0.064
     S3O6-2             0.000e+000  0.000e+000  -183.903  -183.967
-0.064
     S4O6-2             0.000e+000  0.000e+000  -277.572  -277.636
-0.064
     S5O6-2             0.000e+000  0.000e+000  -400.120  -400.184
-0.064
S(5)             0.000e+000
     S2O6-2             0.000e+000  0.000e+000   -74.329   -74.393
-0.064
S(6)             3.986e-005
     SO4-2              3.826e-005  3.302e-005    -4.417    -4.481
-0.064
     CaSO4              8.454e-007  8.454e-007    -6.073    -6.073
0.000
     MgSO4              7.239e-007  7.239e-007    -6.140    -6.140
0.000
     NaSO4-             2.736e-008  2.637e-008    -7.563    -7.579
-0.016
     KSO4-              4.119e-009  3.971e-009    -8.385    -8.401
-0.016
     HSO4-              4.073e-011  3.926e-011   -10.390   -10.406
-0.016
     KHSO4              4.124e-017  4.124e-017   -16.385   -16.385
0.000
     H2SO4              4.360e-022  4.360e-022   -21.360   -21.360
0.000
S(7)             0.000e+000
     S2O8-2             0.000e+000  0.000e+000   -49.008   -49.072
-0.064
S(8)             3.538e-032
     HSO5-              3.538e-032  3.410e-032   -31.451   -31.467
-0.016

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

     Phase               SI log IAP  log KT

     Anhydrite        -3.89   -8.24   -4.35  CaSO4
     Antarcticite    -15.44  -11.34    4.09  CaCl2:6H2O
     Aphthitalite    -23.47  -27.36   -3.89  NaK3(SO4)2
     Aragonite        -1.15    0.82    1.97  CaCO3
     Arcanite        -12.29  -14.13   -1.84  K2SO4
     Artinite         -7.36   12.27   19.63  Mg2CO3(OH)2:3H2O
```

Bassanite	-4.53	-8.24	-3.71	CaSO4:0.5H2O
Bischofite	-16.06	-11.67	4.39	MgCl2:6H2O
Bloedite	-18.41	-20.88	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-4.51	11.77	16.28	Mg(OH)2
Burkeite	-37.37	-27.89	9.49	Na6CO3(SO4)2
C	-71.83	-93.68	-21.85	C
C(g)	-189.45	-93.68	95.77	C
Ca	-125.93	-29.10	96.83	Ca
Ca(g)	-151.17	-29.10	122.07	Ca
Ca2Cl2(OH)2:H2O	-25.53	0.76	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-43.36	24.96	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-1.00	0.82	1.82	CaCO3
Carnallite	-24.56	-20.29	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-4.70	-8.24	-3.54	CaSO4:0.5H2O
CH4(g)	-145.34	-176.08	-30.74	CH4
Chloromagnesite	-33.49	-11.67	21.82	MgCl2
Cl2(g)	-28.23	17.76	45.99	Cl2
CO(g)	-48.16	-52.48	-4.32	CO
CO2(g)	-3.45	-11.28	-7.83	CO2
Dolomite	-1.15	1.32	2.47	CaMg(CO3)2
Dolomite-dis	-2.69	1.32	4.01	CaMg(CO3)2
Dolomite-ord	-1.14	1.32	2.46	CaMg(CO3)2
Epsomite	-6.60	-8.57	-1.96	MgSO4:7H2O
Gaylussite	-13.59	-2.43	11.16	CaNa2(CO3)2:5H2O
Glauberite	-15.09	-20.55	-5.47	Na2Ca(SO4)2
Gypsum	-3.71	-8.24	-4.53	CaSO4:2H2O
H2(g)	-41.20	-41.20	-0.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-143.45	-185.15	-41.70	H2S
Halite	-9.27	-7.71	1.56	NaCl
HCl(g)	-18.02	-11.72	6.30	HCl
Hexahydrite	-6.84	-8.57	-1.73	MgSO4:6H2O
Huntite	-7.91	2.31	10.22	CaMg3(CO3)4
Hydromagnesite	-16.98	13.76	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-23.09	-11.34	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-66.98	-17.50	49.48	K
K(g)	-77.58	-17.50	60.08	K
K2CO3:1.5H2O	-18.45	-5.07	13.38	K2CO3:1.5H2O
K2O	-77.83	6.20	84.04	K2O
K3H(SO4)2	-27.75	-31.37	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-70.55	-42.84	27.71	K8H4(CO3)6:3H2O
Kainite	-16.88	-17.19	-0.31	KMgClSO4:3H2O
Kalicinite	-8.46	-8.17	0.28	KHCO3
Kieserite	-8.30	-8.57	-0.27	MgSO4:H2O
KMgCl3	-41.54	-20.29	21.25	KMgCl3
KMgCl3:2H2O	-34.25	-20.29	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-14.42	-4.16	10.26	KNaCO3:6H2O
Lansfordite	-4.35	0.50	4.84	MgCO3:5H2O
Leonite	-18.59	-22.70	-4.11	K2Mg(SO4)2:4H2O
Lime	-20.47	12.10	32.57	CaO
Magnesite	-1.78	0.50	2.27	MgCO3

```
     Mercallite        -15.80  -17.24   -1.44  KHSO4
     Mg               -108.95  -29.43   79.52  Mg
     Mg(g)            -128.68  -29.43   99.25  Mg
     Mg1.25SO4(OH)0.5:0.5H2O -10.82   -5.62    5.20
Mg1.25SO4(OH)0.5:0.5H2O
     Mg1.5SO4(OH)      -11.89   -2.68    9.21  Mg1.5SO4(OH)
     MgCl2:2H2O        -24.40  -11.67   12.73  MgCl2:2H2O
     MgCl2:4H2O        -18.97  -11.67    7.30  MgCl2:4H2O
     MgCl2:H2O         -27.74  -11.67   16.07  MgCl2:H2O
     MgOHCl            -15.84    0.05   15.89  MgOHCl
     MgSO4             -13.40   -8.57    4.83  MgSO4
     Mirabilite        -11.16  -12.32   -1.15  Na2SO4:10H2O
     Misenite         -106.48 -117.56  -11.08  K8H6(SO4)7
     Monohydrocalcite  -1.85    0.82    2.68  CaCO3:H2O
     Na                -62.46  -16.59   45.87  Na
     Na(g)             -75.95  -16.59   59.36  Na
     Na2CO3            -14.42   -3.25   11.16  Na2CO3
     Na2CO3:7H2O       -13.19   -3.25    9.94  Na2CO3:7H2O
     Na2O              -59.39    8.02   67.42  Na2O
     Na3H(SO4)2        -27.75  -28.64   -0.89  Na3H(SO4)2
     Na4Ca(SO4)3:2H2O -26.98  -32.87   -5.89  Na4Ca(SO4)3:2H2O
     Nahcolite          -7.12   -7.27   -0.14  NaHCO3
     Natron            -12.84   -3.25    9.59  Na2CO3:10H2O
     Nesquehonite       -4.79    0.50    5.29  MgCO3:3H2O
     O2(g)              -0.70   82.40   83.10  O2
     Oxychloride-Mg    -14.01   11.82   25.83  Mg2Cl(OH)3:4H2O
     Pentahydrite       -7.18   -8.57   -1.39  MgSO4:5H2O
     Periclase          -9.55   11.77   21.33  MgO
     Picromerite       -18.26  -22.70   -4.44  K2Mg(SO4)2:6H2O
     Pirssonite        -13.75   -2.43   11.32  Na2Ca(CO3)2:2H2O
     Polyhalite        -24.86  -39.18  -14.31  K2MgCa2(SO4)4:2H2O
     Portlandite       -10.44   12.10   22.55  Ca(OH)2
     S                -108.12 -143.94  -35.82  S
     S2(g)            -230.14 -287.89  -57.75  S2
     SO2(g)            -56.22  -61.54   -5.32  SO2
     Starkeyite         -7.57   -8.57   -1.00  MgSO4:4H2O
     Sylvite            -9.45   -8.62    0.83  KCl
     Syngenite         -14.77  -22.37   -7.60  K2Ca(SO4)2:H2O
     Tachyhydrite      -51.83  -34.68   17.14  Mg2CaCl6:12H2O
     Thenardite        -11.96  -12.32   -0.36  Na2SO4
     Thermonatrite     -14.19   -3.25   10.94  Na2CO3:H2O
     Trona-K           -23.93  -12.34   11.59  K2NaH(CO3)2:2H2O

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

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

     USE SOLUTION  3
```

```
REACTION
NaCN  2.16e-04
NaI   9.49e-07
1.0
EQUILIBRIUM_PHASES 1
Calcite     0.0  6.1
Illite      0.0   4.1
Kaolinite  0.0  0.0
Quartz      0.0  106.5
Gypsum      0.0   0.0013
Albite      0.0  14.4
K-Feldspar  0.0  7.8
Fluorapatite  0.0  0.017
Dolomite  0.0   Enstatite  21.7
Yb2O3  0.0  0.0094
Fe(OH)3  0.0  2.89
Pyrite  0.0  0.17
Zincite  0.0  Sphalerite  0.05
Birnessite  0.0  0.008
Barite  0.0  0.022
Borax  0.0  0.07
PuO2   0.0  8.76e-09
CaUO4  0.0  0.000417
Ca2V2O7  0.0  0.0035
Tb2O3    0.0  0.03
TcO2:2H2O(am)   0.0  5.72e-08
Ca3(AsO4)2  0.0  0.0006
Niter  0.0  0.001
Halite    0.0  0.0009
CaSeO4    0.0  1.8e-04
O2(g)   -0.7   1.0
CO2(g)    -3.5   1.0
END
-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 3.     Solution after simulation 1.
Using pure phase assemblage 1.
Using reaction 1.

Reaction 1.      Irreversible reaction defined in simulation 2.

      1.000e+000 moles of the following reaction have been added:

                        Relative
     Reactant              moles

     NaCN                   0.00
     NaI                    0.00
```

Element	Relative moles
C	0.00
I	0.00
N	0.00
Na	0.00

----------Phase assemblage----------

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Albite	-0.00	2.66	2.66	1.440e+001	1.418e+001	-2.237e-001
Barite	0.00	-10.01	-10.01	2.200e-002	2.200e-002	-1.923e-008
Birnessite	0.00	269.79	269.79	8.000e-003	8.000e-003	-7.028e-014
Borax	0.00	12.04	12.04	7.000e-002	1.221e-002	-5.779e-002
Ca2V2O7	-0.48	16.71	17.18	3.500e-003	-	3.500e-003
Ca3(AsO4)2	-53.49	-35.69	17.80	6.000e-004	-	6.000e-004
Calcite	-0.00	1.82	1.82	6.100e+000	5.975e+000	-1.253e-001
CaSeO4	-4.28	-7.37	-3.09	1.800e-004	-	1.800e-004
CaUO4	-0.00	15.94	15.94	4.170e-004	4.136e-004	-3.407e-006
CO2(g)	-3.50	-11.33	-7.83	1.000e+000	1.063e+000	6.314e-002
Dolomite	-0.00	2.47	2.47			
MgSiO3	is reactant			2.170e+001	2.272e+001	1.024e+000
Fe(OH)3	0.00	18.66	18.66	2.890e+000	3.060e+000	1.700e-001
Fluorapatite	0.00	-25.16	-25.16	1.700e-002	1.580e-002	-1.200e-003
Gypsum	-0.00	-4.53	-4.53	1.300e-003	1.315e-001	1.302e-001
Halite	-5.40	-3.83	1.56	9.000e-004	-	9.000e-004
Illite	-0.40	8.48	8.88	4.100e+000	-	4.100e+000
K-Feldspar	-0.00	-0.38	-0.38	7.800e+000	1.026e+001	2.461e+000

```
     Kaolinite          0.00    6.72    6.72 0.000e+000 3.597e+000
3.597e+000
     Niter             -6.58   -6.81   -0.22 1.000e-003           -
1.000e-003
     O2(g)             -0.70   82.40   83.10 1.000e+000 3.618e-001-
6.382e-001
     PuO2               0.00  -25.93  -25.93 8.760e-009 8.760e-009-
2.901e-013
     Pyrite          -242.00 -325.69  -83.69 1.700e-001           -
1.700e-001
     Quartz             0.00   -4.03   -4.03 1.065e+002 1.059e+002-
5.782e-001
     Tb2O3             -7.09   40.01   47.10 3.000e-002           -
3.000e-002
     TcO2:2H2O(am)    -40.01  -77.23  -37.22 5.720e-008           -
5.720e-008
     Yb2O3             -9.39   38.41   47.80 9.400e-003           -
9.400e-003
     Zincite           -0.00   11.20   11.20
          ZnS             is reactant    5.000e-002 4.988e-002-
1.208e-004

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

     Elements           Molality       Moles

     Al               5.293e-008  4.972e-008
     As               1.277e-003  1.200e-003
     B                2.460e-001  2.311e-001
     Ba               2.047e-008  1.923e-008
     C                6.686e-002  6.281e-002
     Ca               1.094e-002  1.028e-002
     Cl               1.136e-003  1.067e-003
     F                1.277e-003  1.200e-003
     Fe               4.660e-007  4.378e-007
     I                1.010e-006  9.490e-007
     K                3.562e-004  3.346e-004
     Mg               9.261e-004  8.701e-004
     Mn               6.060e-013  5.694e-013
     N                1.294e-003  1.216e-003
     Na               3.625e-001  3.405e-001
     P                3.832e-003  3.600e-003
     Pu               3.088e-013  2.901e-013
     S                2.235e-001  2.100e-001
     Se               1.916e-004  1.800e-004
     Si               1.066e-004  1.002e-004
     Tb               6.386e-002  6.000e-002
     Tc               6.088e-008  5.720e-008
     U                3.626e-006  3.407e-006
     V                7.451e-003  7.000e-003
     Yb               2.001e-002  1.880e-002
```

```
     Zn                1.286e-004  1.208e-004

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

                                        pH  =   8.032      Charge
balance
                                        pe  =  12.571      Adjusted
to redox equilibrium
                         Activity of water  =   0.986
                            Ionic strength  =  5.454e-001
                       Mass of water (kg)   =  9.395e-001
                 Total alkalinity (eq/kg)   =  1.935e-001
                       Total CO2 (mol/kg)   =  6.686e-002
                     Temperature (deg C)    =  25.000
                  Electrical balance (eq)   =  2.197e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =   0.00
                                Iterations  =  44
                                   Total H  = 1.049901e+002
                                   Total O  = 5.392984e+001

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

                                                   Log       Log
Log
     Species            Molality    Activity  Molality  Activity
Gamma

     OH-              1.555e-006  1.023e-006    -5.808    -5.990
-0.182
     H+               1.158e-008  9.281e-009    -7.936    -8.032
-0.096
     H2O              5.553e+001  9.856e-001    -0.006    -0.006
0.000
Al               5.293e-008
     AlO2-            5.062e-008  3.429e-008    -7.296    -7.465
-0.169
     NaAlO2           1.363e-009  1.363e-009    -8.866    -8.866
0.000
     HAlO2            9.289e-010  9.289e-010    -9.032    -9.032
0.000
     Al(OH)2+         8.747e-012  5.924e-012   -11.058   -11.227
-0.169
     AlOH+2           1.203e-013  2.402e-014   -12.920   -13.619
-0.700
     Al(SO4)2-        1.404e-015  9.508e-016   -14.853   -15.022
-0.169
     AlSO4+           7.428e-016  5.031e-016   -15.129   -15.298
-0.169
     Al+3             2.238e-016  2.019e-017   -15.650   -16.695
-1.045
```

```
     AlHPO4+            1.197e-016  8.108e-017   -15.922   -16.091
-0.169
     Al2(OH)2+4         3.447e-023  9.384e-026   -22.463   -25.028
-2.565
     AlF+2              4.640e-024  9.267e-025   -23.334   -24.033
-0.700
     AlH2PO4+2          1.888e-028  3.772e-029   -27.724   -28.423
-0.700
     Al3(OH)4+5         9.127e-029  1.379e-032   -28.040   -31.860
-3.821
     AlF2+              2.500e-033  1.693e-033   -32.602   -32.771
-0.169
     AlF3               0.000e+000  0.000e+000   -43.009   -43.009
0.000
     Al13O4(OH)24+7     0.000e+000  0.000e+000   -51.392   -58.902
-7.510
     AlF4-              0.000e+000  0.000e+000   -54.778   -54.948
-0.169
As(-3)          0.000e+000
     AsH3               0.000e+000  0.000e+000  -185.600  -185.600
0.000
As(3)           0.000e+000
     HAsO2              0.000e+000  0.000e+000   -57.042   -57.042
0.000
     As(OH)3            0.000e+000  0.000e+000   -57.107   -57.107
0.000
     H2AsO3-            0.000e+000  0.000e+000   -58.118   -58.288
-0.169
     AsO2-              0.000e+000  0.000e+000   -58.132   -58.301
-0.169
     AsO2OH-2           0.000e+000  0.000e+000   -60.521   -61.265
-0.744
     HAsS2              0.000e+000  0.000e+000  -333.373  -333.373
0.000
As(5)           1.277e-003
     AsO3F-2            1.275e-003  2.299e-004    -2.895    -3.639
-0.744
     HAsO3F-            2.339e-006  1.584e-006    -5.631    -5.800
-0.169
     HAsO4-2            2.785e-028  5.021e-029   -27.555   -28.299
-0.744
     H2AsO4-            4.145e-030  2.807e-030   -29.382   -29.552
-0.169
     AsO4-3             6.988e-031  1.388e-032   -30.156   -31.858
-1.702
     H3AsO4             4.589e-036  4.589e-036   -35.338   -35.338
0.000
B(-5)           0.000e+000
     BH4-               0.000e+000  0.000e+000  -222.362  -222.531
-0.169
B(3)            2.460e-001
```

```
     B(OH)3            2.201e-001  2.201e-001    -0.657    -0.657
0.000
     BO2-              1.905e-002  1.290e-002    -1.720    -1.889
-0.169
     NaB(OH)4          5.169e-003  5.169e-003    -2.287    -2.287
0.000
     CaB(OH)4+         1.624e-003  1.100e-003    -2.790    -2.959
-0.169
     MgB(OH)4+         1.288e-004  8.725e-005    -3.890    -4.059
-0.169
     BaB(OH)4+         2.177e-009  1.475e-009    -8.662    -8.831
-0.169
     B2O(OH)5-         1.591e-012  1.077e-012   -11.798   -11.968
-0.169
     BF2(OH)2-         2.671e-031  1.809e-031   -30.573   -30.743
-0.169
     BF3OH-            0.000e+000  0.000e+000   -46.308   -46.477
-0.169
     BF4-              0.000e+000  0.000e+000   -63.851   -64.020
-0.169
Ba               2.047e-008
     Ba+2              1.825e-008  3.993e-009    -7.739    -8.399
-0.660
     BaB(OH)4+         2.177e-009  1.475e-009    -8.662    -8.831
-0.169
     BaNO3+            3.832e-011  2.595e-011   -10.417   -10.586
-0.169
     BaCO3             4.646e-012  4.646e-012   -11.333   -11.333
0.000
     BaCl+             1.396e-012  9.457e-013   -11.855   -12.024
-0.169
     BaOH+             2.121e-014  1.437e-014   -13.673   -13.843
-0.169
     BaF+              1.864e-023  1.262e-023   -22.730   -22.899
-0.169
C(-2)            0.000e+000
     C2H4              0.000e+000  0.000e+000  -266.310  -266.310
0.000
C(-3)            0.000e+000
     C2H6              0.000e+000  0.000e+000  -238.631  -238.631
0.000
C(-4)            0.000e+000
     CH4               0.000e+000  0.000e+000  -148.248  -148.248
0.000
C(2)             0.000e+000
     CO                0.000e+000  0.000e+000   -51.206   -51.206
0.000
C(4)             6.686e-002
     TbCO3+            2.686e-002  1.820e-002    -1.571    -1.740
-0.169
     YbCO3+            9.874e-003  6.688e-003    -2.005    -2.175
-0.169
```

Tb(CO3)2-	9.716e-003	6.580e-003	-2.013	-2.182	-0.169
Yb(CO3)2-	4.867e-003	3.296e-003	-2.313	-2.482	-0.169
HCO3-	7.357e-004	4.983e-004	-3.133	-3.303	-0.169
NaHCO3	1.485e-004	1.485e-004	-3.828	-3.828	0.000
CO3-2	1.193e-005	2.382e-006	-4.924	-5.623	-0.700
TbHCO3+2	1.097e-005	2.191e-006	-4.960	-5.659	-0.700
CaHCO3+	1.084e-005	7.345e-006	-4.965	-5.134	-0.169
CO2	9.594e-006	1.088e-005	-5.018	-4.963	0.055
CaCO3	6.867e-006	6.867e-006	-5.163	-5.163	0.000
UO2(CO3)3-4	3.427e-006	3.103e-009	-5.465	-8.508	-3.043
NaCO3-	2.564e-006	1.736e-006	-5.591	-5.760	-0.169
YbHCO3+2	2.413e-006	4.819e-007	-5.618	-6.317	-0.700
MgHCO3+	7.087e-007	4.800e-007	-6.150	-6.319	-0.169
ZnCO3	2.765e-007	2.765e-007	-6.558	-6.558	0.000
ZnHCO3+	2.621e-007	1.775e-007	-6.582	-6.751	-0.169
MgCO3	2.090e-007	2.090e-007	-6.680	-6.680	0.000
UO2(CO3)2-2	1.606e-007	2.896e-008	-6.794	-7.538	-0.744
(UO2)2CO3(OH)3-	1.589e-009	1.076e-009	-8.799	-8.968	-0.169
UO2CO3	6.320e-010	6.320e-010	-9.199	-9.199	0.000
BaCO3	4.646e-012	4.646e-012	-11.333	-11.333	0.000
(UO2)3(CO3)6-6	2.592e-013	3.457e-020	-12.586	-19.461	-6.875
PuO2(CO3)2-2	2.396e-013	4.320e-014	-12.620	-13.364	-0.744
FeCO3+	7.391e-015	5.006e-015	-14.131	-14.301	-0.169
MnCO3	4.895e-015	4.895e-015	-14.310	-14.310	0.000
MnHCO3+	3.288e-016	2.227e-016	-15.483	-15.652	-0.169
FeHCO3+	3.931e-019	2.663e-019	-18.405	-18.575	-0.169

```
     FeCO3              1.377e-019  1.377e-019   -18.861   -18.861
0.000
     (UO2)3(OH)5CO2+  3.324e-021  2.251e-021   -20.478   -20.648
-0.169
     (UO2)3O(OH)2(HCO3)+  2.719e-021  1.842e-021   -20.566   -
20.735    -0.169
     UO2(CO3)3-5        9.239e-030  1.578e-034   -29.034   -33.802
-4.767
     U(CO3)4-4          0.000e+000  0.000e+000   -45.777   -48.820
-3.043
     (UO2)11(CO3)6(OH)12-2  0.000e+000  0.000e+000   -46.342   -
47.086    -0.744
     U(CO3)5-6          0.000e+000  0.000e+000   -48.651   -55.526
-6.875
     SCN-               0.000e+000  0.000e+000  -214.854  -215.036
-0.182
     UO2SCN+            0.000e+000  0.000e+000  -226.733  -226.902
-0.169
     USCN+3             0.000e+000  0.000e+000  -272.031  -273.544
-1.513
     Zn(SCN)2           0.000e+000  0.000e+000  -434.051  -434.051
0.000
     UO2(SCN)2          0.000e+000  0.000e+000  -442.106  -442.106
0.000
     U(SCN)2+2          0.000e+000  0.000e+000  -486.579  -487.279
-0.700
     UO2(SCN)3-         0.000e+000  0.000e+000  -656.113  -656.282
-0.169
     Zn(SCN)4-2         0.000e+000  0.000e+000  -863.012  -863.756
-0.744
Ca                1.094e-002
     Ca+2               4.868e-003  1.244e-003    -2.313    -2.905
-0.593
     CaSO4              4.424e-003  4.424e-003    -2.354    -2.354
0.000
     CaB(OH)4+          1.624e-003  1.100e-003    -2.790    -2.959
-0.169
     CaHCO3+            1.084e-005  7.345e-006    -4.965    -5.134
-0.169
     CaNO3+             7.533e-006  5.102e-006    -5.123    -5.292
-0.169
     CaCO3              6.867e-006  6.867e-006    -5.163    -5.163
0.000
     CaCl+              2.749e-007  1.862e-007    -6.561    -6.730
-0.169
     CaHPO4             1.093e-007  1.093e-007    -6.961    -6.961
0.000
     CaPO4-             4.349e-008  2.946e-008    -7.362    -7.531
-0.169
     CaOH+              2.755e-008  1.866e-008    -7.560    -7.729
-0.169
```

```
     CaCl2              1.546e-010  1.546e-010    -9.811    -9.811
0.000
     CaP2O7-2           2.025e-013  3.650e-014   -12.694   -13.438
-0.744
     CaH2PO4+           6.845e-017  4.636e-017   -16.165   -16.334
-0.169
     CaF+               4.285e-017  2.902e-017   -16.368   -16.537
-0.169
Cl(-1)          1.136e-003
     Cl-                1.109e-003  7.061e-004    -2.955    -3.151
-0.196
     NaCl               2.585e-005  2.585e-005    -4.587    -4.587
0.000
     TbCl+2             5.296e-007  1.058e-007    -6.276    -6.976
-0.700
     CaCl+              2.749e-007  1.862e-007    -6.561    -6.730
-0.169
     YbCl+2             7.096e-008  1.417e-008    -7.149    -7.849
-0.700
     MgCl+              6.751e-008  4.572e-008    -7.171    -7.340
-0.169
     Zn(OH)Cl           2.977e-008  2.977e-008    -7.526    -7.526
0.000
     ZnCl+              2.421e-008  1.640e-008    -7.616    -7.785
-0.169
     KCl                4.538e-009  4.538e-009    -8.343    -8.343
0.000
     CaCl2              1.546e-010  1.546e-010    -9.811    -9.811
0.000
     TbCl2+             6.037e-011  4.089e-011   -10.219   -10.388
-0.169
     ZnCl2              1.352e-011  1.352e-011   -10.869   -10.869
0.000
     YbCl2+             5.854e-012  3.965e-012   -11.233   -11.402
-0.169
     HCl                1.472e-012  1.472e-012   -11.832   -11.832
0.000
     BaCl+              1.396e-012  9.457e-013   -11.855   -12.024
-0.169
     TbCl3              1.132e-014  1.132e-014   -13.946   -13.946
0.000
     ZnCl3-             7.785e-015  5.273e-015   -14.109   -14.278
-0.169
     YbCl3              8.967e-016  8.967e-016   -15.047   -15.047
0.000
     ZnCl4-2            1.565e-016  2.822e-017   -15.805   -16.549
-0.744
     MnCl+              1.303e-016  8.826e-017   -15.885   -16.054
-0.169
     UO2Cl+             8.201e-017  5.554e-017   -16.086   -16.255
-0.169
```

```
     TbCl4-          4.334e-018  2.935e-018   -17.363   -17.532
-0.169
     YbCl4-          3.463e-019  2.345e-019   -18.461   -18.630
-0.169
     PuO2Cl+         5.367e-021  3.635e-021   -20.270   -20.439
-0.169
     UO2Cl2          2.008e-021  2.008e-021   -20.697   -20.697
0.000
     FeCl+           7.733e-022  5.237e-022   -21.112   -21.281
-0.169
     FeCl+2          2.143e-022  4.281e-023   -21.669   -22.368
-0.700
     FeCl2+          3.613e-023  2.447e-023   -22.442   -22.611
-0.169
     MnCl3-          1.419e-023  9.611e-024   -22.848   -23.017
-0.169
     FeCl2           1.984e-027  1.984e-027   -26.702   -26.702
0.000
     FeCl4-          2.165e-032  1.467e-032   -31.664   -31.834
-0.169
     FeCl4-2         1.585e-032  2.858e-033   -31.800   -32.544
-0.744
     UCl+3           0.000e+000  0.000e+000   -61.407   -62.920
-1.513
Cl(1)          1.592e-020
     ClO-            1.291e-020  8.744e-021   -19.889   -20.058
-0.169
     HClO            3.009e-021  3.009e-021   -20.522   -20.522
0.000
Cl(3)          2.038e-030
     ClO2-           2.038e-030  1.380e-030   -29.691   -29.860
-0.169
     HClO2           1.894e-035  1.894e-035   -34.723   -34.723
0.000
Cl(5)          2.357e-026
     ClO3-           2.357e-026  1.550e-026   -25.628   -25.810
-0.182
     UO2ClO3+        3.880e-039  2.628e-039   -38.411   -38.580
-0.169
Cl(7)          1.322e-026
     ClO4-           1.321e-026  8.694e-027   -25.879   -26.061
-0.182
     ZnClO4+         3.356e-030  2.273e-030   -29.474   -29.643
-0.169
F              1.277e-003
     AsO3F-2         1.275e-003  2.299e-004    -2.895    -3.639
-0.744
     HAsO3F-         2.339e-006  1.584e-006    -5.631    -5.800
-0.169
     TbF+2           9.275e-014  1.852e-014   -13.033   -13.732
-0.700
```

YbF+2	2.065e-014	4.124e-015	-13.685	-14.385	-0.700
F-	6.976e-015	4.590e-015	-14.156	-14.338	-0.182
NaF	1.023e-016	1.023e-016	-15.990	-15.990	0.000
CaF+	4.285e-017	2.902e-017	-16.368	-16.537	-0.169
MgF+	1.357e-017	9.188e-018	-16.868	-17.037	-0.169
ZnF+	1.323e-018	8.961e-019	-17.878	-18.048	-0.169
HF	6.539e-020	6.539e-020	-19.184	-19.184	0.000
PO3F-2	6.064e-022	1.093e-022	-21.217	-21.961	-0.744
UO2F+	4.224e-023	2.861e-023	-22.374	-22.543	-0.169
BaF+	1.864e-023	1.262e-023	-22.730	-22.899	-0.169
AlF+2	4.640e-024	9.267e-025	-23.334	-24.033	-0.700
VO2F	1.523e-024	1.523e-024	-23.817	-23.817	0.000
TbF2+	4.048e-025	2.742e-025	-24.393	-24.562	-0.169
YbF2+	1.073e-025	7.270e-026	-24.969	-25.138	-0.169
PuO2F+	2.660e-026	1.802e-026	-25.575	-25.744	-0.169
HPO3F-	1.884e-026	1.276e-026	-25.725	-25.894	-0.169
MnF+	1.071e-026	7.252e-027	-25.970	-26.140	-0.169
FeF+2	1.254e-028	2.505e-029	-27.902	-28.601	-0.700
BF2(OH)2-	2.671e-031	1.809e-031	-30.573	-30.743	-0.169
FeF+	1.581e-031	1.071e-031	-30.801	-30.970	-0.169
AlF2+	2.500e-033	1.693e-033	-32.602	-32.771	-0.169
H2PO3F	7.574e-034	7.574e-034	-33.121	-33.121	0.000
UO2F2	3.941e-034	3.941e-034	-33.404	-33.404	0.000
HF2-	1.073e-034	7.270e-035	-33.969	-34.138	-0.169
VOF+	1.935e-035	1.310e-035	-34.713	-34.883	-0.169
PuO2F2	1.634e-035	1.634e-035	-34.787	-34.787	0.000

VO2F2-	2.977e-036	2.016e-036	-35.526	-35.696	-0.169
TbF3	4.612e-037	4.612e-037	-36.336	-36.336	0.000
YbF3	1.657e-037	1.657e-037	-36.781	-36.781	0.000
H2F2	1.064e-038	1.064e-038	-37.973	-37.973	0.000
FeF2+	2.747e-039	1.860e-039	-38.561	-38.730	-0.169
AlF3	0.000e+000	0.000e+000	-43.009	-43.009	0.000
PuF+3	0.000e+000	0.000e+000	-43.844	-45.356	-1.513
PuO2F3-	0.000e+000	0.000e+000	-43.990	-44.159	-0.169
UO2F3-	0.000e+000	0.000e+000	-45.307	-45.476	-0.169
BF3OH-	0.000e+000	0.000e+000	-46.308	-46.477	-0.169
VOF2	0.000e+000	0.000e+000	-46.441	-46.441	0.000
TbF4-	0.000e+000	0.000e+000	-48.429	-48.598	-0.169
YbF4-	0.000e+000	0.000e+000	-48.777	-48.946	-0.169
PuF2+2	0.000e+000	0.000e+000	-52.055	-52.755	-0.700
AlF4-	0.000e+000	0.000e+000	-54.778	-54.948	-0.169
PuO2F4-2	0.000e+000	0.000e+000	-54.880	-55.624	-0.744
UO2F4-2	0.000e+000	0.000e+000	-58.295	-59.039	-0.744
BF4-	0.000e+000	0.000e+000	-63.851	-64.020	-0.169
UF+3	0.000e+000	0.000e+000	-65.050	-66.563	-1.513
UF2+2	0.000e+000	0.000e+000	-73.275	-73.975	-0.700
PuF3+	0.000e+000	0.000e+000	-77.024	-77.193	-0.169
UF3+	0.000e+000	0.000e+000	-82.792	-82.962	-0.169
PuF4	0.000e+000	0.000e+000	-92.631	-92.631	0.000
UF4	0.000e+000	0.000e+000	-93.356	-93.356	0.000
SiF6-2	0.000e+000	0.000e+000	-95.043	-95.787	-0.744
UF5-	0.000e+000	0.000e+000	-106.197	-106.366	-0.169

```
     UF6-2              0.000e+000  0.000e+000  -117.930  -118.674
-0.744
Fe(2)            8.497e-018
     Fe+2               3.984e-018  1.018e-018   -17.400   -17.992
-0.593
     FeSO4              3.929e-018  3.929e-018   -17.406   -17.406
0.000
     FeHCO3+            3.931e-019  2.663e-019   -18.405   -18.575
-0.169
     FeCO3              1.377e-019  1.377e-019   -18.861   -18.861
0.000
     FeOH+              5.049e-020  3.419e-020   -19.297   -19.466
-0.169
     FePO4-             1.051e-021  7.115e-022   -20.979   -21.148
-0.169
     FeCl+              7.733e-022  5.237e-022   -21.112   -21.281
-0.169
     FeHPO4             6.480e-022  6.480e-022   -21.188   -21.188
0.000
     Fe(OH)2            2.885e-023  2.885e-023   -22.540   -22.540
0.000
     Fe(OH)3-           1.801e-025  1.220e-025   -24.745   -24.914
-0.169
     FeCl2              1.984e-027  1.984e-027   -26.702   -26.702
0.000
     FeH2PO4+           1.118e-030  7.571e-031   -29.952   -30.121
-0.169
     FeF+               1.581e-031  1.071e-031   -30.801   -30.970
-0.169
     Fe(OH)4-2          7.183e-032  1.295e-032   -31.144   -31.888
-0.744
     FeCl4-2            1.585e-032  2.858e-033   -31.800   -32.544
-0.744
Fe(3)            4.660e-007
     Fe(OH)3            4.359e-007  4.359e-007    -6.361    -6.361
0.000
     Fe(OH)4-           1.717e-008  1.163e-008    -7.765    -7.935
-0.169
     Fe(OH)2+           1.296e-008  8.774e-009    -7.888    -8.057
-0.169
     FeOH+2             1.249e-012  2.495e-013   -11.903   -12.603
-0.700
     FeCO3+             7.391e-015  5.006e-015   -14.131   -14.301
-0.169
     FeHPO4+            1.300e-015  8.805e-016   -14.886   -15.055
-0.169
     Fe+3               4.033e-018  3.639e-019   -17.394   -18.439
-1.045
     FeSO4+             1.266e-018  8.572e-019   -17.898   -18.067
-0.169
     Fe(SO4)2-          5.210e-019  3.529e-019   -18.283   -18.452
-0.169
```

```
     FeNO3+2          1.491e-020  2.978e-021   -19.827   -20.526
-0.700
     Fe2(OH)2+4       6.154e-022  1.676e-024   -21.211   -23.776
-2.565
     FeCl+2           2.143e-022  4.281e-023   -21.669   -22.368
-0.700
     FeCl2+           3.613e-023  2.447e-023   -22.442   -22.611
-0.169
     Fe3(OH)4+5       2.032e-026  3.072e-030   -25.692   -29.513
-3.821
     FeF+2            1.254e-028  2.505e-029   -27.902   -28.601
-0.700
     FeH2PO4+2        3.998e-029  7.986e-030   -28.398   -29.098
-0.700
     FeNO2+2          7.702e-032  1.538e-032   -31.113   -31.813
-0.700
     FeCl4-           2.165e-032  1.467e-032   -31.664   -31.834
-0.169
     FeF2+            2.747e-039  1.860e-039   -38.561   -38.730
-0.169
H(0)            0.000e+000
     H2               0.000e+000  0.000e+000   -44.363   -44.308
0.055
I(-03)          0.000e+000
     I3-              0.000e+000  0.000e+000   -48.263   -48.432
-0.169
I(-1)           5.662e-019
     I-               5.639e-019  3.590e-019   -18.249   -18.445
-0.196
     NaI              2.251e-021  2.251e-021   -20.648   -20.648
0.000
     KI               1.776e-024  1.776e-024   -23.751   -23.751
0.000
     ZnI+             7.103e-027  4.811e-027   -26.149   -26.318
-0.169
     ZnI2             0.000e+000  0.000e+000   -43.593   -43.593
0.000
     ZnI3-            0.000e+000  0.000e+000   -62.030   -62.200
-0.169
     UI+3             0.000e+000  0.000e+000   -77.203   -78.716
-1.513
     ZnI4-2           0.000e+000  0.000e+000   -80.500   -81.244
-0.744
I(1)            1.033e-021
     IO-              1.033e-021  6.996e-022   -20.986   -21.155
-0.169
I(5)            1.010e-006
     IO3-             1.010e-006  6.841e-007    -5.996    -6.165
-0.169
     HIO3             1.969e-014  1.969e-014   -13.706   -13.706
0.000
```

```
     UO2IO3+          2.824e-018  1.913e-018   -17.549   -17.718
-0.169
     UO2(IO3)2        2.457e-023  2.457e-023   -22.610   -22.610
0.000
I(7)            3.191e-019
     IO4-             3.191e-019  2.100e-019   -18.496   -18.678
-0.182
K               3.562e-004
     K+               3.006e-004  1.914e-004    -3.522    -3.718
-0.196
     KSO4-            5.553e-005  3.761e-005    -4.255    -4.425
-0.169
     KCl              4.538e-009  4.538e-009    -8.343    -8.343
0.000
     KHPO4-           2.722e-010  1.844e-010    -9.565    -9.734
-0.169
     KOH              7.047e-011  7.047e-011   -10.152   -10.152
0.000
     KHSO4            3.080e-013  3.080e-013   -12.511   -12.511
0.000
     KP2O7-3          1.065e-017  2.116e-019   -16.973   -18.674
-1.702
     KI               1.776e-024  1.776e-024   -23.751   -23.751
0.000
Mg              9.261e-004
     MgSO4            5.393e-004  5.393e-004    -3.268    -3.268
0.000
     Mg+2             2.569e-004  8.294e-005    -3.590    -4.081
-0.491
     MgB(OH)4+        1.288e-004  8.725e-005    -3.890    -4.059
-0.169
     MgHCO3+          7.087e-007  4.800e-007    -6.150    -6.319
-0.169
     MgCO3            2.090e-007  2.090e-007    -6.680    -6.680
0.000
     MgCl+            6.751e-008  4.572e-008    -7.171    -7.340
-0.169
     MgHPO4           1.078e-008  1.078e-008    -7.967    -7.967
0.000
     MgPO4-           3.903e-009  2.643e-009    -8.409    -8.578
-0.169
     MgP2O7-2         3.997e-014  7.207e-015   -13.398   -14.142
-0.744
     MgF+             1.357e-017  9.188e-018   -16.868   -17.037
-0.169
     MgH2PO4+         8.306e-018  5.625e-018   -17.081   -17.250
-0.169
     Mg4(OH)4+4       3.933e-022  1.071e-024   -21.405   -23.970
-2.565
Mn(2)           5.887e-013
     MnSO4            3.527e-013  3.527e-013   -12.453   -12.453
0.000
```

```
     Mn+2              2.297e-013  5.870e-014   -12.639   -13.231
-0.593
     MnCO3             4.895e-015  4.895e-015   -14.310   -14.310
0.000
     MnSeO4            5.456e-016  5.456e-016   -15.263   -15.263
0.000
     MnHCO3+           3.288e-016  2.227e-016   -15.483   -15.652
-0.169
     MnOH+             2.366e-016  1.603e-016   -15.626   -15.795
-0.169
     MnCl+             1.303e-016  8.826e-017   -15.885   -16.054
-0.169
     MnNO3+            1.124e-016  7.614e-017   -15.949   -16.118
-0.169
     MnHPO4            3.568e-017  3.568e-017   -16.448   -16.448
0.000
     MnPO4-            1.102e-017  7.465e-018   -16.958   -17.127
-0.169
     Mn(NO3)2          1.565e-019  1.565e-019   -18.805   -18.805
0.000
     MnH2PO4+          4.620e-020  3.129e-020   -19.335   -19.505
-0.169
     Mn(OH)2           4.178e-020  4.178e-020   -19.379   -19.379
0.000
     MnCl3-            1.419e-023  9.611e-024   -22.848   -23.017
-0.169
     Mn(OH)3-          6.144e-024  4.162e-024   -23.212   -23.381
-0.169
     MnF+              1.071e-026  7.252e-027   -25.970   -26.140
-0.169
     Mn2(OH)3+         7.673e-027  5.197e-027   -26.115   -26.284
-0.169
     Mn2OH+3           3.283e-028  1.008e-029   -27.484   -28.997
-1.513
     Mn(OH)4-2         2.076e-029  3.743e-030   -28.683   -29.427
-0.744
Mn(3)            1.901e-025
     Mn+3              1.901e-025  5.836e-027   -24.721   -26.234
-1.513
Mn(6)            3.851e-017
     MnO4-2            3.851e-017  6.943e-018   -16.414   -17.158
-0.744
Mn(7)            1.732e-014
     MnO4-             1.732e-014  1.140e-014   -13.761   -13.943
-0.182
N(-03)           0.000e+000
     N3-               0.000e+000  0.000e+000  -100.039  -100.208
-0.169
     HN3               0.000e+000  0.000e+000  -103.538  -103.538
0.000
     ZnN3+             0.000e+000  0.000e+000  -104.456  -104.625
-0.169
```

```
      UO2N3+            0.000e+000  0.000e+000  -110.736  -110.905
-0.169
      Zn(N3)2           0.000e+000  0.000e+000  -204.080  -204.080
0.000
      UO2(N3)2          0.000e+000  0.000e+000  -209.363  -209.363
0.000
      UO2(N3)3-         0.000e+000  0.000e+000  -307.991  -308.161
-0.169
      UO2(N3)4-2        0.000e+000  0.000e+000  -408.445  -409.189
-0.744
N(-3)             0.000e+000
      NH4+              0.000e+000  0.000e+000   -64.589   -64.802
-0.213
      NH3               0.000e+000  0.000e+000   -66.009   -66.009
0.000
      Zn(NH3)+2         0.000e+000  0.000e+000   -68.116   -68.816
-0.700
      NH4SO4-           0.000e+000  0.000e+000   -74.546   -74.715
-0.169
      Zn(NH3)2+2        0.000e+000  0.000e+000  -131.919  -132.619
-0.700
      Zn(NH3)3+2        0.000e+000  0.000e+000  -195.722  -196.421
-0.700
      SCN-              0.000e+000  0.000e+000  -214.854  -215.036
-0.182
      UO2SCN+           0.000e+000  0.000e+000  -226.733  -226.902
-0.169
      Zn(NH3)4+2        0.000e+000  0.000e+000  -259.798  -260.498
-0.700
      USCN+3            0.000e+000  0.000e+000  -272.031  -273.544
-1.513
      Zn(SCN)2          0.000e+000  0.000e+000  -434.051  -434.051
0.000
      UO2(SCN)2         0.000e+000  0.000e+000  -442.106  -442.106
0.000
      U(SCN)2+2         0.000e+000  0.000e+000  -486.579  -487.279
-0.700
      UO2(SCN)3-        0.000e+000  0.000e+000  -656.113  -656.282
-0.169
      Zn(SCN)4-2        0.000e+000  0.000e+000  -863.012  -863.756
-0.744
N(-5)             0.000e+000
      HCN               0.000e+000  0.000e+000  -122.324  -122.324
0.000
      CN-               0.000e+000  0.000e+000  -123.354  -123.550
-0.196
      Zn(CN)4-2         0.000e+000  0.000e+000  -481.542  -482.286
-0.744
N(0)              2.354e-021
      N2                1.177e-021  1.177e-021   -20.929   -20.929
0.000
N(3)              4.702e-017
```

```
     NO2-              4.702e-017  2.993e-017   -16.328   -16.524
-0.196
     HNO2              4.741e-022  4.741e-022   -21.324   -21.324
0.000
     FeNO2+2           7.702e-032  1.538e-032   -31.113   -31.813
-0.700
N(5)             1.294e-003
     NO3-              1.285e-003  8.183e-004    -2.891    -3.087
-0.196
     CaNO3+            7.533e-006  5.102e-006    -5.123    -5.292
-0.169
     TbNO3+2           1.157e-006  2.312e-007    -5.937    -6.636
-0.700
     YbNO3+2           9.307e-008  1.859e-008    -7.031    -7.731
-0.700
     BaNO3+            3.832e-011  2.595e-011   -10.417   -10.586
-0.169
     HNO3              3.972e-013  3.972e-013   -12.401   -12.401
0.000
     UO2NO3+           1.219e-016  8.255e-017   -15.914   -16.083
-0.169
     MnNO3+            1.124e-016  7.614e-017   -15.949   -16.118
-0.169
     Mn(NO3)2          1.565e-019  1.565e-019   -18.805   -18.805
0.000
     FeNO3+2           1.491e-020  2.978e-021   -19.827   -20.526
-0.700
     UNO3+3            0.000e+000  0.000e+000   -61.610   -63.123
-1.513
     U(NO3)2+2         0.000e+000  0.000e+000   -64.700   -65.400
-0.700
Na               3.625e-001
     Na+               3.076e-001  2.083e-001    -0.512    -0.681
-0.169
     NaSO4-            4.949e-002  3.352e-002    -1.306    -1.475
-0.169
     NaB(OH)4          5.169e-003  5.169e-003    -2.287    -2.287
0.000
     NaHCO3            1.485e-004  1.485e-004    -3.828    -3.828
0.000
     NaCl              2.585e-005  2.585e-005    -4.587    -4.587
0.000
     NaHSiO3           1.117e-005  1.117e-005    -4.952    -4.952
0.000
     NaCO3-            2.564e-006  1.736e-006    -5.591    -5.760
-0.169
     NaHPO4-           4.091e-007  2.771e-007    -6.388    -6.557
-0.169
     NaOH              3.678e-008  3.678e-008    -7.434    -7.434
0.000
     NaAlO2            1.363e-009  1.363e-009    -8.866    -8.866
0.000
```

```
     Na2P2O7-2          1.734e-014  3.127e-015   -13.761   -14.505
-0.744
     NaP2O7-3           9.512e-015  1.889e-016   -14.022   -15.724
-1.702
     NaHP2O7-2          1.968e-015  3.548e-016   -14.706   -15.450
-0.744
     NaF                1.023e-016  1.023e-016   -15.990   -15.990
0.000
     NaI                2.251e-021  2.251e-021   -20.648   -20.648
0.000
O(0)             4.507e-004
     O2                 2.254e-004  2.556e-004    -3.647    -3.592
0.055
     UO2S2O3            0.000e+000  0.000e+000  -156.680  -156.680
0.000
     S3O6-2             0.000e+000  0.000e+000  -175.021  -175.765
-0.744
     S2-2               0.000e+000  0.000e+000  -249.276  -250.020
-0.744
     S4O6-2             0.000e+000  0.000e+000  -266.022  -266.766
-0.744
     S3-2               0.000e+000  0.000e+000  -353.700  -354.444
-0.744
     S5O6-2             0.000e+000  0.000e+000  -385.902  -386.646
-0.744
     S4-2               0.000e+000  0.000e+000  -458.351  -459.095
-0.744
     S5-2               0.000e+000  0.000e+000  -563.218  -563.962
-0.744
P(-3)            0.000e+000
     PH4+               0.000e+000  0.000e+000  -236.280  -236.450
-0.169
P(5)             3.832e-003
     TbPO4              1.700e-003  1.700e-003    -2.770    -2.770
0.000
     YbPO4              8.515e-004  8.515e-004    -3.070    -3.070
0.000
     Yb(PO4)2-3         3.519e-004  6.990e-006    -3.454    -5.156
-1.702
     Tb(PO4)2-3         2.797e-004  5.556e-006    -3.553    -5.255
-1.702
     TbHPO4+            1.228e-005  8.315e-006    -4.911    -5.080
-0.169
     YbHPO4+            3.082e-006  2.087e-006    -5.511    -5.680
-0.169
     HPO4-2             8.867e-007  1.599e-007    -6.052    -6.796
-0.744
     NaHPO4-            4.091e-007  2.771e-007    -6.388    -6.557
-0.169
     CaHPO4             1.093e-007  1.093e-007    -6.961    -6.961
0.000
```

CaPO4-	4.349e-008	2.946e-008	-7.362	-7.531	-0.169
H2PO4-	3.705e-008	2.509e-008	-7.431	-7.600	-0.169
ZnPO4-	1.755e-008	1.188e-008	-7.756	-7.925	-0.169
Tb(HPO4)2-	1.559e-008	1.056e-008	-7.807	-7.976	-0.169
MgHPO4	1.078e-008	1.078e-008	-7.967	-7.967	0.000
Yb(HPO4)2-	7.809e-009	5.289e-009	-8.107	-8.277	-0.169
ZnHPO4	4.021e-009	4.021e-009	-8.396	-8.396	0.000
MgPO4-	3.903e-009	2.643e-009	-8.409	-8.578	-0.169
TbH2PO4+2	1.628e-009	3.252e-010	-8.788	-9.488	-0.700
PO4-3	3.931e-010	7.807e-012	-9.406	-11.107	-1.702
YbH2PO4+2	3.591e-010	7.172e-011	-9.445	-10.144	-0.700
KHPO4-	2.722e-010	1.844e-010	-9.565	-9.734	-0.169
UO2PO4-	1.616e-010	1.095e-010	-9.792	-9.961	-0.169
UO2HPO4	2.327e-012	2.327e-012	-11.633	-11.633	0.000
CaP2O7-2	2.025e-013	3.650e-014	-12.694	-13.438	-0.744
MgP2O7-2	3.997e-014	7.207e-015	-13.398	-14.142	-0.744
H3PO4	3.588e-014	3.588e-014	-13.445	-13.445	0.000
VO2HPO4-	2.365e-014	1.602e-014	-13.626	-13.795	-0.169
Na2P2O7-2	1.734e-014	3.127e-015	-13.761	-14.505	-0.744
NaP2O7-3	9.512e-015	1.889e-016	-14.022	-15.724	-1.702
P2O7-4	5.559e-015	5.034e-018	-14.255	-17.298	-3.043
HP2O7-3	3.839e-015	7.626e-017	-14.416	-16.118	-1.702
NaHP2O7-2	1.968e-015	3.548e-016	-14.706	-15.450	-0.744
FeHPO4+	1.300e-015	8.805e-016	-14.886	-15.055	-0.169
AlHPO4+	1.197e-016	8.108e-017	-15.922	-16.091	-0.169
VO2(HPO4)2-3	7.593e-017	1.508e-018	-16.120	-17.822	-1.702

CaH2PO4+	6.845e-017	4.636e-017	-16.165	-16.334	-0.169
UO2H2PO4+	5.442e-017	3.686e-017	-16.264	-16.433	-0.169
MnHPO4	3.568e-017	3.568e-017	-16.448	-16.448	0.000
H2P2O7-2	1.624e-017	2.927e-018	-16.790	-17.534	-0.744
MnPO4-	1.102e-017	7.465e-018	-16.958	-17.127	-0.169
KP2O7-3	1.065e-017	2.116e-019	-16.973	-18.674	-1.702
MgH2PO4+	8.306e-018	5.625e-018	-17.081	-17.250	-0.169
ZnH2PO4+	8.149e-020	5.519e-020	-19.089	-19.258	-0.169
MnH2PO4+	4.620e-020	3.129e-020	-19.335	-19.505	-0.169
Pu(HPO4)4-4	5.760e-021	5.216e-024	-20.240	-23.283	-3.043
PuO2H2PO4+	3.108e-021	2.105e-021	-20.508	-20.677	-0.169
FePO4-	1.051e-021	7.115e-022	-20.979	-21.148	-0.169
FeHPO4	6.480e-022	6.480e-022	-21.188	-21.188	0.000
UO2(H2PO4)2	6.452e-022	6.452e-022	-21.190	-21.190	0.000
PO3F-2	6.064e-022	1.093e-022	-21.217	-21.961	-0.744
H3P2O7-	9.219e-024	6.244e-024	-23.035	-23.205	-0.169
UO2H3PO4+2	7.476e-025	1.493e-025	-24.126	-24.826	-0.700
Pu(HPO4)3-2	2.646e-026	4.770e-027	-25.577	-26.321	-0.744
HPO3F-	1.884e-026	1.276e-026	-25.725	-25.894	-0.169
VO2H2PO4	1.053e-026	1.053e-026	-25.978	-25.978	0.000
AlH2PO4+2	1.888e-028	3.772e-029	-27.724	-28.423	-0.700
UO2(H2PO4)(H3PO4)+	9.047e-029	6.127e-029	-28.043	-28.213	-0.169
FeH2PO4+2	3.998e-029	7.986e-030	-28.398	-29.098	-0.700
Pu(HPO4)2	6.556e-030	6.556e-030	-29.183	-29.183	0.000
H4P2O7	1.703e-030	1.703e-030	-29.769	-29.769	0.000
FeH2PO4+	1.118e-030	7.571e-031	-29.952	-30.121	-0.169

```
      PuHPO4+2          2.968e-033  5.929e-034   -32.527   -33.227
-0.700
      H2PO3F            7.574e-034  7.574e-034   -33.121   -33.121
0.000
      PuH2PO4+2         3.472e-040  0.000e+000   -39.459   -40.159
-0.700
Pu(3)            1.752e-032
      Pu(SO4)2-         1.612e-032  1.092e-032   -31.793   -31.962
-0.169
      PuSO4+            1.062e-033  7.192e-034   -32.974   -33.143
-0.169
      Pu+3              2.871e-034  8.816e-036   -33.542   -35.055
-1.513
      PuOH+2            5.022e-035  1.003e-035   -34.299   -34.999
-0.700
      PuH2PO4+2         3.472e-040  0.000e+000   -39.459   -40.159
-0.700
Pu(4)            1.376e-017
      Pu(OH)4           1.375e-017  1.375e-017   -16.862   -16.862
0.000
      Pu(HPO4)4-4       5.760e-021  5.216e-024   -20.240   -23.283
-3.043
      Pu(OH)3+          3.020e-021  2.046e-021   -20.520   -20.689
-0.169
      Pu(OH)2+2         8.891e-026  1.776e-026   -25.051   -25.751
-0.700
      Pu(HPO4)3-2       2.646e-026  4.770e-027   -25.577   -26.321
-0.744
      Pu(HPO4)2         6.556e-030  6.556e-030   -29.183   -29.183
0.000
      PuOH+3            3.603e-031  1.106e-032   -30.443   -31.956
-1.513
      Pu(SO4)2          3.730e-033  3.730e-033   -32.428   -32.428
0.000
      PuHPO4+2          2.968e-033  5.929e-034   -32.527   -33.227
-0.700
      PuSO4+2           2.596e-035  5.186e-036   -34.586   -35.285
-0.700
      Pu+4              1.221e-037  3.325e-040   -36.913   -39.478
-2.565
      PuF+3             0.000e+000  0.000e+000   -43.844   -45.356
-1.513
      PuF2+2            0.000e+000  0.000e+000   -52.055   -52.755
-0.700
      PuF3+             0.000e+000  0.000e+000   -77.024   -77.193
-0.169
      PuF4              0.000e+000  0.000e+000   -92.631   -92.631
0.000
Pu(5)            6.585e-014
      PuO2+             6.483e-014  4.391e-014   -13.188   -13.357
-0.169
```

```
     PuO2OH              1.021e-015  1.021e-015   -14.991   -14.991
0.000
Pu(6)            2.429e-013
     PuO2(CO3)2-2        2.396e-013  4.320e-014   -12.620   -13.364
-0.744
     PuO2OH+             2.901e-015  1.965e-015   -14.537   -14.707
-0.169
     PuO2SO4             3.719e-016  3.719e-016   -15.430   -15.430
0.000
     PuO2+2              4.035e-017  8.060e-018   -16.394   -17.094
-0.700
     PuO2Cl+             5.367e-021  3.635e-021   -20.270   -20.439
-0.169
     PuO2H2PO4+          3.108e-021  2.105e-021   -20.508   -20.677
-0.169
     PuO2F+              2.660e-026  1.802e-026   -25.575   -25.744
-0.169
     (PuO2)2(OH)2+2      2.011e-026  4.016e-027   -25.697   -26.396
-0.700
     (PuO2)3(OH)5+       2.295e-033  1.555e-033   -32.639   -32.808
-0.169
     PuO2F2              1.634e-035  1.634e-035   -34.787   -34.787
0.000
     PuO2F3-             0.000e+000  0.000e+000   -43.990   -44.159
-0.169
     PuO2F4-2            0.000e+000  0.000e+000   -54.880   -55.624
-0.744
S(-2)            0.000e+000
     HS-                 0.000e+000  0.000e+000  -140.562  -140.744
-0.182
     H2S                 0.000e+000  0.000e+000  -141.767  -141.767
0.000
     S-2                 0.000e+000  0.000e+000  -144.977  -145.637
-0.660
     SCN-                0.000e+000  0.000e+000  -214.854  -215.036
-0.182
     UO2SCN+             0.000e+000  0.000e+000  -226.733  -226.902
-0.169
     S2-2                0.000e+000  0.000e+000  -249.276  -250.020
-0.744
     USCN+3              0.000e+000  0.000e+000  -272.031  -273.544
-1.513
     HAsS2               0.000e+000  0.000e+000  -333.373  -333.373
0.000
     S3-2                0.000e+000  0.000e+000  -353.700  -354.444
-0.744
     Zn(SCN)2            0.000e+000  0.000e+000  -434.051  -434.051
0.000
     UO2(SCN)2           0.000e+000  0.000e+000  -442.106  -442.106
0.000
     S4-2                0.000e+000  0.000e+000  -458.351  -459.095
-0.744
```

```
     U(SCN)2+2          0.000e+000  0.000e+000  -486.579  -487.279
-0.700
     S5-2               0.000e+000  0.000e+000  -563.218  -563.962
-0.744
     UO2(SCN)3-         0.000e+000  0.000e+000  -656.113  -656.282
-0.169
     Zn(SCN)4-2         0.000e+000  0.000e+000  -863.012  -863.756
-0.744
S(2)             0.000e+000
     S2O3-2             0.000e+000  0.000e+000  -144.831  -145.575
-0.744
     HS2O3-             0.000e+000  0.000e+000  -152.424  -152.593
-0.169
S(3)             0.000e+000
     S2O4-2             0.000e+000  0.000e+000  -134.135  -134.795
-0.660
S(4)             0.000e+000
     SO3-2              0.000e+000  0.000e+000   -45.736   -46.435
-0.700
     HSO3-              0.000e+000  0.000e+000   -47.067   -47.236
-0.169
     UO2SO3             0.000e+000  0.000e+000   -52.959   -52.959
0.000
     H2SO3              0.000e+000  0.000e+000   -53.287   -53.287
0.000
     SO2                0.000e+000  0.000e+000   -53.381   -53.381
0.000
     UO2(SO3)2-2        0.000e+000  0.000e+000   -97.493   -98.237
-0.744
     S2O5-2             0.000e+000  0.000e+000   -98.552   -99.296
-0.744
     UO2S2O3            0.000e+000  0.000e+000  -156.680  -156.680
0.000
     S3O6-2             0.000e+000  0.000e+000  -175.021  -175.765
-0.744
     S4O6-2             0.000e+000  0.000e+000  -266.022  -266.766
-0.744
     S5O6-2             0.000e+000  0.000e+000  -385.902  -386.646
-0.744
S(5)             0.000e+000
     S2O6-2             0.000e+000  0.000e+000   -68.114   -68.858
-0.744
S(6)             2.235e-001
     SO4-2              1.350e-001  2.435e-002    -0.870    -1.614
-0.744
     NaSO4-             4.949e-002  3.352e-002    -1.306    -1.475
-0.169
     TbSO4+             1.463e-002  9.907e-003    -1.835    -2.004
-0.169
     Tb(SO4)2-          7.215e-003  4.887e-003    -2.142    -2.311
-0.169
```

CaSO4	4.424e-003	4.424e-003	-2.354	-2.354	0.000
YbSO4+	1.960e-003	1.328e-003	-2.708	-2.877	-0.169
Yb(SO4)2-	1.439e-003	9.745e-004	-2.842	-3.011	-0.169
MgSO4	5.393e-004	5.393e-004	-3.268	-3.268	0.000
ZnSO4	7.071e-005	7.071e-005	-4.151	-4.151	0.000
KSO4-	5.553e-005	3.761e-005	-4.255	-4.425	-0.169
HSO4-	3.370e-008	2.283e-008	-7.472	-7.642	-0.169
UO2(SO4)2-2	1.873e-012	3.377e-013	-11.727	-12.471	-0.744
UO2SO4	1.565e-012	1.565e-012	-11.805	-11.805	0.000
MnSO4	3.527e-013	3.527e-013	-12.453	-12.453	0.000
KHSO4	3.080e-013	3.080e-013	-12.511	-12.511	0.000
VO2SO4-	2.026e-013	1.372e-013	-12.693	-12.863	-0.169
Al(SO4)2-	1.404e-015	9.508e-016	-14.853	-15.022	-0.169
AlSO4+	7.428e-016	5.031e-016	-15.129	-15.298	-0.169
PuO2SO4	3.719e-016	3.719e-016	-15.430	-15.430	0.000
FeSO4	3.929e-018	3.929e-018	-17.406	-17.406	0.000
FeSO4+	1.266e-018	8.572e-019	-17.898	-18.067	-0.169
Fe(SO4)2-	5.210e-019	3.529e-019	-18.283	-18.452	-0.169
H2SO4	1.999e-019	1.999e-019	-18.699	-18.699	0.000
VOSO4	2.099e-024	2.099e-024	-23.678	-23.678	0.000
Pu(SO4)2-	1.612e-032	1.092e-032	-31.793	-31.962	-0.169
Pu(SO4)2	3.730e-033	3.730e-033	-32.428	-32.428	0.000
PuSO4+	1.062e-033	7.192e-034	-32.974	-33.143	-0.169
PuSO4+2	2.596e-035	5.186e-036	-34.586	-35.285	-0.700
VSO4+	0.000e+000	0.000e+000	-45.493	-45.662	-0.169
U(SO4)2	0.000e+000	0.000e+000	-54.339	-54.339	0.000

```
     USO4+2            0.000e+000  0.000e+000   -55.866   -56.565
-0.700
     NH4SO4-           0.000e+000  0.000e+000   -74.546   -74.715
-0.169
S(7)             0.000e+000
     S2O8-2            0.000e+000  0.000e+000   -42.793   -43.537
-0.744
S(8)             2.927e-029
     HSO5-             2.927e-029  1.983e-029   -28.534   -28.703
-0.169
Se(-2)           0.000e+000
     HSe-              0.000e+000  0.000e+000   -95.931   -96.100
-0.169
     H2Se              0.000e+000  0.000e+000  -100.311  -100.311
0.000
     Se-2              0.000e+000  0.000e+000  -102.270  -103.014
-0.744
Se(4)            1.314e-016
     SeO3-2            1.251e-016  2.256e-017   -15.903   -16.647
-0.744
     HSeO3-            6.352e-018  4.302e-018   -17.197   -17.366
-0.169
     H2SeO3            1.517e-023  1.517e-023   -22.819   -22.819
0.000
Se(6)            1.916e-004
     SeO4-2            1.915e-004  3.453e-005    -3.718    -4.462
-0.744
     ZnSeO4            7.392e-008  7.392e-008    -7.131    -7.131
0.000
     HSeO4-            4.024e-011  2.725e-011   -10.395   -10.565
-0.169
     MnSeO4            5.456e-016  5.456e-016   -15.263   -15.263
0.000
Si               1.066e-004
     SiO2              9.379e-005  9.379e-005    -4.028    -4.028
0.000
     NaHSiO3           1.117e-005  1.117e-005    -4.952    -4.952
0.000
     HSiO3-            1.680e-006  1.138e-006    -5.775    -5.944
-0.169
     H2SiO4-2          6.433e-011  1.160e-011   -10.192   -10.936
-0.744
     H6(H2SiO4)4-2     1.017e-013  1.833e-014   -12.993   -13.737
-0.744
     H4(H2SiO4)4-4     1.178e-017  1.066e-020   -16.929   -19.972
-3.043
     SiF6-2            0.000e+000  0.000e+000   -95.043   -95.787
-0.744
Tb(2)            0.000e+000
     Tb+2              0.000e+000  0.000e+000   -73.232   -73.932
-0.700
Tb(3)            6.386e-002
```

```
     TbCO3+            2.686e-002  1.820e-002    -1.571    -1.740
-0.169
     TbSO4+            1.463e-002  9.907e-003    -1.835    -2.004
-0.169
     Tb(CO3)2-         9.716e-003  6.580e-003    -2.013    -2.182
-0.169
     Tb(SO4)2-         7.215e-003  4.887e-003    -2.142    -2.311
-0.169
     Tb+3              2.685e-003  8.243e-005    -2.571    -4.084
-1.513
     TbPO4             1.700e-003  1.700e-003    -2.770    -2.770
0.000
     TbOH+2            6.496e-004  1.298e-004    -3.187    -3.887
-0.700
     Tb(PO4)2-3        2.797e-004  5.556e-006    -3.553    -5.255
-1.702
     TbO+              9.052e-005  6.130e-005    -4.043    -4.213
-0.169
     TbHPO4+           1.228e-005  8.315e-006    -4.911    -5.080
-0.169
     TbHCO3+2          1.097e-005  2.191e-006    -4.960    -5.659
-0.700
     TbO2H             8.679e-006  8.679e-006    -5.062    -5.062
0.000
     TbNO3+2           1.157e-006  2.312e-007    -5.937    -6.636
-0.700
     TbO2-             9.494e-007  6.430e-007    -6.023    -6.192
-0.169
     TbCl+2            5.296e-007  1.058e-007    -6.276    -6.976
-0.700
     Tb(HPO4)2-        1.559e-008  1.056e-008    -7.807    -7.976
-0.169
     TbH2PO4+2         1.628e-009  3.252e-010    -8.788    -9.488
-0.700
     TbCl2+            6.037e-011  4.089e-011   -10.219   -10.388
-0.169
     TbF+2             9.275e-014  1.852e-014   -13.033   -13.732
-0.700
     TbCl3             1.132e-014  1.132e-014   -13.946   -13.946
0.000
     TbCl4-            4.334e-018  2.935e-018   -17.363   -17.532
-0.169
     TbF2+             4.048e-025  2.742e-025   -24.393   -24.562
-0.169
     TbF3              4.612e-037  4.612e-037   -36.336   -36.336
0.000
     TbF4-             0.000e+000  0.000e+000   -48.429   -48.598
-0.169
Tc(3)            0.000e+000
     Tc+3              0.000e+000  0.000e+000   -82.011   -83.523
-1.513
Tc(4)            0.000e+000
```

```
     TcO(OH)2          0.000e+000  0.000e+000   -47.554   -47.554
0.000
     TcOOH+            0.000e+000  0.000e+000   -53.224   -53.394
-0.169
     TcO+2             0.000e+000  0.000e+000   -59.585   -60.284
-0.700
     (TcO(OH)2)2       0.000e+000  0.000e+000   -88.591   -88.591
0.000
Tc(5)            0.000e+000
     TcO4-3            0.000e+000  0.000e+000   -51.117   -52.819
-1.702
Tc(6)            6.619e-030
     HTcO4-            3.688e-030  2.498e-030   -29.433   -29.602
-0.169
     TcO4-2            2.930e-030  5.283e-031   -29.533   -30.277
-0.744
     H2TcO4            4.602e-038  4.602e-038   -37.337   -37.337
0.000
Tc(7)            6.088e-008
     TcO4-             6.088e-008  4.123e-008    -7.216    -7.385
-0.169
U(3)             0.000e+000
     U+3               0.000e+000  0.000e+000   -81.895   -83.408
-1.513
U(4)             1.199e-034
     U(OH)4            1.199e-034  1.199e-034   -33.921   -33.921
0.000
     U(CO3)4-4         0.000e+000  0.000e+000   -45.777   -48.820
-3.043
     U(CO3)5-6         0.000e+000  0.000e+000   -48.651   -55.526
-6.875
     UOH+3             0.000e+000  0.000e+000   -52.493   -54.006
-1.513
     U(SO4)2           0.000e+000  0.000e+000   -54.339   -54.339
0.000
     USO4+2            0.000e+000  0.000e+000   -55.866   -56.565
-0.700
     U+4               0.000e+000  0.000e+000   -58.921   -61.486
-2.565
     UCl+3             0.000e+000  0.000e+000   -61.407   -62.920
-1.513
     UNO3+3            0.000e+000  0.000e+000   -61.610   -63.123
-1.513
     U(NO3)2+2         0.000e+000  0.000e+000   -64.700   -65.400
-0.700
     UF+3              0.000e+000  0.000e+000   -65.050   -66.563
-1.513
     UF2+2             0.000e+000  0.000e+000   -73.275   -73.975
-0.700
     UI+3              0.000e+000  0.000e+000   -77.203   -78.716
-1.513
```

```
     UF3+                0.000e+000  0.000e+000   -82.792   -82.962
-0.169
     UF4                 0.000e+000  0.000e+000   -93.356   -93.356
0.000
     UF5-                0.000e+000  0.000e+000  -106.197  -106.366
-0.169
     UF6-2               0.000e+000  0.000e+000  -117.930  -118.674
-0.744
     USCN+3              0.000e+000  0.000e+000  -272.031  -273.544
-1.513
     U(SCN)2+2           0.000e+000  0.000e+000  -486.579  -487.279
-0.700
U(5)             6.337e-025
     UO2+                6.337e-025  4.292e-025   -24.198   -24.367
-0.169
     UO2(CO3)3-5         9.239e-030  1.578e-034   -29.034   -33.802
-4.767
U(6)             3.626e-006
     UO2(CO3)3-4         3.427e-006  3.103e-009    -5.465    -8.508
-3.043
     UO2(CO3)2-2         1.606e-007  2.896e-008    -6.794    -7.538
-0.744
     UO2(OH)2            2.890e-008  2.890e-008    -7.539    -7.539
0.000
     UO2(OH)3-           5.612e-009  3.801e-009    -8.251    -8.420
-0.169
      (UO2)2CO3(OH)3-    1.589e-009  1.076e-009    -8.799    -8.968
-0.169
     UO2CO3              6.320e-010  6.320e-010    -9.199    -9.199
0.000
     UO2PO4-             1.616e-010  1.095e-010    -9.792    -9.961
-0.169
     UO2OH+              5.132e-011  3.476e-011   -10.290   -10.459
-0.169
     UO2HPO4             2.327e-012  2.327e-012   -11.633   -11.633
0.000
     UO2(SO4)2-2         1.873e-012  3.377e-013   -11.727   -12.471
-0.744
     UO2SO4              1.565e-012  1.565e-012   -11.805   -11.805
0.000
     UO2+2               2.647e-013  5.288e-014   -12.577   -13.277
-0.700
      (UO2)3(CO3)6-6     2.592e-013  3.457e-020   -12.586   -19.461
-6.875
     UO2(OH)4-2          3.489e-014  6.291e-015   -13.457   -14.201
-0.744
      (UO2)3(OH)7-       2.959e-015  2.004e-015   -14.529   -14.698
-0.169
      (UO2)3(OH)5+       7.513e-016  5.089e-016   -15.124   -15.293
-0.169
      (UO2)2(OH)2+2      3.671e-016  7.332e-017   -15.435   -16.135
-0.700
```

```
     UO2NO3+            1.219e-016  8.255e-017   -15.914   -16.083
-0.169
     UO2Cl+             8.201e-017  5.554e-017   -16.086   -16.255
-0.169
     UO2H2PO4+          5.442e-017  3.686e-017   -16.264   -16.433
-0.169
     UO2IO3+            2.824e-018  1.913e-018   -17.549   -17.718
-0.169
     (UO2)4(OH)7+       1.970e-019  1.334e-019   -18.706   -18.875
-0.169
     (UO2)3(OH)4+2      1.109e-019  2.215e-020   -18.955   -19.655
-0.700
     (UO2)2OH+3         1.898e-020  5.828e-022   -19.722   -21.235
-1.513
     (UO2)3(OH)5CO2+    3.324e-021  2.251e-021   -20.478   -20.648
-0.169
     (UO2)3O(OH)2(HCO3)+  2.719e-021  1.842e-021   -20.566   -
20.735    -0.169
     UO2Cl2             2.008e-021  2.008e-021   -20.697   -20.697
0.000
     UO2(H2PO4)2        6.452e-022  6.452e-022   -21.190   -21.190
0.000
     UO2F+              4.224e-023  2.861e-023   -22.374   -22.543
-0.169
     UO2(IO3)2          2.457e-023  2.457e-023   -22.610   -22.610
0.000
     UO2H3PO4+2         7.476e-025  1.493e-025   -24.126   -24.826
-0.700
     UO2(H2PO4)(H3PO4)+  9.047e-029  6.127e-029   -28.043   -28.213
-0.169
     UO2F2              3.941e-034  3.941e-034   -33.404   -33.404
0.000
     UO2ClO3+           3.880e-039  2.628e-039   -38.411   -38.580
-0.169
     UO2F3-             0.000e+000  0.000e+000   -45.307   -45.476
-0.169
     (UO2)11(CO3)6(OH)12-2  0.000e+000  0.000e+000   -46.342   -
47.086    -0.744
     UO2SO3             0.000e+000  0.000e+000   -52.959   -52.959
0.000
     UO2F4-2            0.000e+000  0.000e+000   -58.295   -59.039
-0.744
     UO2(SO3)2-2        0.000e+000  0.000e+000   -97.493   -98.237
-0.744
     UO2N3+             0.000e+000  0.000e+000  -110.736  -110.905
-0.169
     UO2S2O3            0.000e+000  0.000e+000  -156.680  -156.680
0.000
     UO2(N3)2           0.000e+000  0.000e+000  -209.363  -209.363
0.000
     UO2SCN+            0.000e+000  0.000e+000  -226.733  -226.902
-0.169
```

```
     UO2(N3)3-          0.000e+000  0.000e+000  -307.991  -308.161
-0.169
     UO2(N3)4-2         0.000e+000  0.000e+000  -408.445  -409.189
-0.744
     UO2(SCN)2          0.000e+000  0.000e+000  -442.106  -442.106
0.000
     UO2(SCN)3-         0.000e+000  0.000e+000  -656.113  -656.282
-0.169
V(3)            8.392e-038
     V(OH)2+            8.392e-038  5.684e-038   -37.076   -37.245
-0.169
     VOH+2              0.000e+000  0.000e+000   -40.913   -41.612
-0.700
     VSO4+              0.000e+000  0.000e+000   -45.493   -45.662
-0.169
     V+3                0.000e+000  0.000e+000   -45.865   -47.378
-1.513
     V2(OH)2+4          0.000e+000  0.000e+000   -79.939   -82.504
-2.565
V(4)            9.923e-023
     VOOH+              9.571e-023  6.482e-023   -22.019   -22.188
-0.169
     VOSO4              2.099e-024  2.099e-024   -23.678   -23.678
0.000
     VO+2               1.429e-024  2.855e-025   -23.845   -24.544
-0.700
     VOF+               1.935e-035  1.310e-035   -34.713   -34.883
-0.169
     (VO)2(OH)2+2       9.839e-040  1.965e-040   -39.007   -39.707
-0.700
     VOF2               0.000e+000  0.000e+000   -46.441   -46.441
0.000
V(5)            7.451e-003
     VO3OH-2            6.487e-003  1.170e-003    -2.188    -2.932
-0.744
     HVO4-2             6.458e-004  1.164e-004    -3.190    -3.934
-0.744
     H2VO4-             1.937e-004  1.312e-004    -3.713    -3.882
-0.169
     VO2(OH)2-          1.237e-004  8.378e-005    -3.908    -4.077
-0.169
     VO4-3              3.487e-008  6.926e-010    -7.458    -9.160
-1.702
     VO(OH)3            7.776e-009  7.776e-009    -8.109    -8.109
0.000
     VO2+               2.188e-013  1.482e-013   -12.660   -12.829
-0.169
     VO2SO4-            2.026e-013  1.372e-013   -12.693   -12.863
-0.169
     VO2HPO4-           2.365e-014  1.602e-014   -13.626   -13.795
-0.169
```

```
     VO2(HPO4)2-3      7.593e-017  1.508e-018   -16.120   -17.822
-1.702
     VO2F              1.523e-024  1.523e-024   -23.817   -23.817
0.000
     VO2H2PO4          1.053e-026  1.053e-026   -25.978   -25.978
0.000
     VO2F2-            2.977e-036  2.016e-036   -35.526   -35.696
-0.169
Yb(2)            1.960e-035
     Yb+2              1.960e-035  3.914e-036   -34.708   -35.407
-0.700
Yb(3)            2.001e-002
     YbCO3+            9.874e-003  6.688e-003    -2.005    -2.175
-0.169
     Yb(CO3)2-         4.867e-003  3.296e-003    -2.313    -2.482
-0.169
     YbSO4+            1.960e-003  1.328e-003    -2.708    -2.877
-0.169
     Yb(SO4)2-         1.439e-003  9.745e-004    -2.842    -3.011
-0.169
     YbPO4             8.515e-004  8.515e-004    -3.070    -3.070
0.000
     Yb+3              4.253e-004  1.306e-005    -3.371    -4.884
-1.513
     Yb(PO4)2-3        3.519e-004  6.990e-006    -3.454    -5.156
-1.702
     YbOH+2            1.706e-004  3.408e-005    -3.768    -4.468
-0.700
     YbO+              3.912e-005  2.650e-005    -4.408    -4.577
-0.169
     YbO2H             2.083e-005  2.083e-005    -4.681    -4.681
0.000
     YbO2-             5.189e-006  3.514e-006    -5.285    -5.454
-0.169
     YbHPO4+           3.082e-006  2.087e-006    -5.511    -5.680
-0.169
     YbHCO3+2          2.413e-006  4.819e-007    -5.618    -6.317
-0.700
     YbNO3+2           9.307e-008  1.859e-008    -7.031    -7.731
-0.700
     YbCl+2            7.096e-008  1.417e-008    -7.149    -7.849
-0.700
     Yb(HPO4)2-        7.809e-009  5.289e-009    -8.107    -8.277
-0.169
     YbH2PO4+2         3.591e-010  7.172e-011    -9.445   -10.144
-0.700
     YbCl2+            5.854e-012  3.965e-012   -11.233   -11.402
-0.169
     YbF+2             2.065e-014  4.124e-015   -13.685   -14.385
-0.700
     YbCl3             8.967e-016  8.967e-016   -15.047   -15.047
0.000
```

```
     YbCl4-            3.463e-019  2.345e-019   -18.461   -18.630
-0.169
     YbF2+             1.073e-025  7.270e-026   -24.969   -25.138
-0.169
     YbF3              1.657e-037  1.657e-037   -36.781   -36.781
0.000
     YbF4-             0.000e+000  0.000e+000   -48.777   -48.946
-0.169
Zn                1.286e-004
     ZnSO4             7.071e-005  7.071e-005    -4.151    -4.151
0.000
     Zn+2              5.408e-005  1.382e-005    -4.267    -4.859
-0.593
     ZnOH+             2.377e-006  1.610e-006    -5.624    -5.793
-0.169
     Zn(OH)2           7.322e-007  7.322e-007    -6.135    -6.135
0.000
     ZnCO3             2.765e-007  2.765e-007    -6.558    -6.558
0.000
     ZnHCO3+           2.621e-007  1.775e-007    -6.582    -6.751
-0.169
     ZnSeO4            7.392e-008  7.392e-008    -7.131    -7.131
0.000
     Zn(OH)Cl          2.977e-008  2.977e-008    -7.526    -7.526
0.000
     ZnCl+             2.421e-008  1.640e-008    -7.616    -7.785
-0.169
     ZnPO4-            1.755e-008  1.188e-008    -7.756    -7.925
-0.169
     ZnHPO4            4.021e-009  4.021e-009    -8.396    -8.396
0.000
     Zn(OH)3-          3.558e-010  2.410e-010    -9.449    -9.618
-0.169
     ZnCl2             1.352e-011  1.352e-011   -10.869   -10.869
0.000
     Zn(OH)4-2         2.420e-014  4.364e-015   -13.616   -14.360
-0.744
     ZnCl3-            7.785e-015  5.273e-015   -14.109   -14.278
-0.169
     ZnCl4-2           1.565e-016  2.822e-017   -15.805   -16.549
-0.744
     ZnF+              1.323e-018  8.961e-019   -17.878   -18.048
-0.169
     ZnH2PO4+          8.149e-020  5.519e-020   -19.089   -19.258
-0.169
     ZnI+              7.103e-027  4.811e-027   -26.149   -26.318
-0.169
     ZnClO4+           3.356e-030  2.273e-030   -29.474   -29.643
-0.169
     ZnI2              0.000e+000  0.000e+000   -43.593   -43.593
0.000
```

```
     ZnI3-              0.000e+000  0.000e+000   -62.030   -62.200
-0.169
     Zn(NH3)+2          0.000e+000  0.000e+000   -68.116   -68.816
-0.700
     ZnI4-2             0.000e+000  0.000e+000   -80.500   -81.244
-0.744
     ZnN3+              0.000e+000  0.000e+000  -104.456  -104.625
-0.169
     Zn(NH3)2+2         0.000e+000  0.000e+000  -131.919  -132.619
-0.700
     Zn(NH3)3+2         0.000e+000  0.000e+000  -195.722  -196.421
-0.700
     Zn(N3)2            0.000e+000  0.000e+000  -204.080  -204.080
0.000
     Zn(NH3)4+2         0.000e+000  0.000e+000  -259.798  -260.498
-0.700
     Zn(SCN)2           0.000e+000  0.000e+000  -434.051  -434.051
0.000
     Zn(CN)4-2          0.000e+000  0.000e+000  -481.542  -482.286
-0.744
     Zn(SCN)4-2         0.000e+000  0.000e+000  -863.012  -863.756
-0.744

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

     Phase                SI log IAP  log KT

     (UO2)2As2O7      -77.27  -69.59    7.68  (UO2)2As2O7
     (UO2)2Cl3        -59.78  -48.58   11.20  (UO2)2Cl3
     (UO2)2P2O7       -25.37  -40.14  -14.77  (UO2)2P2O7
     (UO2)3(AsO4)2    -76.10  -66.80    9.29  (UO2)3(AsO4)2
     (UO2)3(PO4)2     -23.26  -37.36  -14.10  (UO2)3(PO4)2
     (UO2)3(PO4)2:4H2O -10.33  -37.38  -27.05  (UO2)3(PO4)2:4H2O
     (VO)3(PO4)2     -119.95 -121.90   -1.96  (VO)3(PO4)2
     Afwillite        -28.58   31.39   59.96  Ca3Si2O4(OH)6
     Akermanite       -15.00   30.23   45.23  Ca2MgSi2O7
     Al              -139.83  -54.41   85.42  Al
     Al(g)           -190.53  -54.41  136.12  Al
     Al2(SO4)3        -57.13  -38.23   18.90  Al2(SO4)3
     Al2(SO4)3:6H2O   -39.82  -38.27    1.56  Al2(SO4)3:6H2O
     Alabandite      -145.52 -179.65  -34.13  MnS
     Albite            -0.00    2.66    2.66  NaAlSi3O8
     Albite_high       -1.32    2.66    3.98  NaAlSi3O8
     Albite_low        -0.00    2.66    2.66  NaAlSi3O8
     AlF3             -42.44  -59.71  -17.27  AlF3
     Alstonite         -4.43   -1.84    2.58  BaCa(CO3)2
     Alum-K           -18.74  -23.72   -4.97  KAl(SO4)2:12H2O
     Alunite           -8.40   -8.87   -0.47  KAl3(OH)6(SO4)2
     Amesite-14A       -5.87   69.40   75.27  Mg4Al4Si2O10(OH)8
     Analcime          -0.13    5.93    6.06  Na.96Al.96Si2.04O6:H2O
     Analcime-dehy     -6.49    5.93   12.42  Na.96Al.96Si2.04O6
```

Andalusite	-5.12	10.76	15.88	Al2SiO5
Andradite	5.49	64.71	59.22	Ca3Fe2(SiO4)3
Anhydrite	-0.17	-4.52	-4.35	CaSO4
Annite	-35.52	-6.19	29.33	KFe3AlSi3O10(OH)2
Anorthite	-6.59	19.88	26.48	CaAl2(SiO4)2
Antarcticite	-13.34	-9.25	4.09	CaCl2:6H2O
Anthophyllite	-14.87	51.61	66.48	Mg7Si8O22(OH)2
Antigorite	-37.86	437.77	475.63	Mg48Si34O85(OH)62
Aphthitalite	-11.17	-15.06	-3.89	NaK3(SO4)2
Aragonite	-0.15	1.82	1.97	CaCO3
Arcanite	-7.21	-9.05	-1.84	K2SO4
Arsenolite	-112.78	-157.55	-44.77	As2O3
Arsenopyrite	-262.21	-324.99	-62.78	FeAsS
Artinite	-7.03	12.60	19.63	Mg2CO3(OH)2:3H2O
As	-106.30	-140.58	-34.28	As
As2O5	-77.28	-75.15	2.14	As2O5
As4O6(cubi)	-225.42	-315.10	-89.69	As4O6
As4O6(mono)	-225.19	-315.10	-89.91	As4O6
Autunite-H	-14.79	-40.15	-25.35	H2(UO2)2(PO4)2
B	-107.51	-62.45	45.06	B
B(g)	-198.80	-62.45	136.35	B
B2O3	-6.84	-1.30	5.55	B2O3
Ba	-131.77	-33.54	98.23	Ba
Ba(OH)2:8H2O	-16.89	7.60	24.49	Ba(OH)2:8H2O
Ba2Si3O8	-19.99	3.24	23.23	Ba2Si3O8
Ba2SiO4	-33.26	11.29	44.55	Ba2SiO4
Ba2U2O7	-53.81	-20.32	33.49	Ba2U2O7
Ba3UO6	-68.60	25.76	94.36	Ba3UO6
BaCl2	-16.93	-14.70	2.23	BaCl2
BaCl2:2H2O	-14.92	-14.71	0.21	BaCl2:2H2O
BaCl2:H2O	-15.53	-14.71	0.82	BaCl2:H2O
BaHPO4	-7.79	-15.19	-7.40	BaHPO4
BaI2	-56.33	-267.94	-211.61	BaI2
BaMnO4	-15.47	92.89	108.36	BaMnO4
BaO	-40.14	7.66	47.80	BaO
Barite	0.00	-10.01	-10.01	BaSO4
Barytocalcite	-4.59	-1.84	2.74	BaCa(CO3)2
BaS	-157.35	-174.82	-17.47	BaS
BaSeO3	-18.47	-54.06	-35.59	BaSeO3
BaSeO4	-5.40	-12.86	-7.46	BaSeO4
BaSiF6	-98.36	-130.57	-32.22	BaSiF6
Bassanite	-0.82	-4.52	-3.71	CaSO4:0.5H2O
Bassetite	-24.33	-42.07	-17.74	Fe(UO2)2(PO4)2
BaU2O7	-8.74	13.22	21.96	BaU2O7
BaUO4	-7.75	10.44	18.19	BaUO4
Beidellite-Ca	-0.84	4.61	5.44	Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H	-2.05	2.44	4.49	H.33Al2.33Si3.67O10(OH)2
Beidellite-K	-1.30	3.86	5.16	K.33Al2.33Si3.67O10(OH)2

Beidellite-Mg	-0.99	4.41	5.41	Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na	-0.64	4.86	5.50	Na.33Al2.33Si3.67O10(OH)2
Berlinite	-8.19	-15.46	-7.27	AlPO4
BF3(g)	-64.77	-67.75	-2.98	BF3
Birnessite	0.00	269.79	269.79	Mn8O14:5H2O
Bischofite	-14.81	-10.42	4.39	MgCl2:6H2O
Bixbyite	-3.33	46.86	50.18	Mn2O3
Bloedite	-6.22	-8.70	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-0.16	7.39	7.55	AlO2H
Boltwoodite	-11.83	3.06	14.89	K(H3O)(UO2)SiO4
Boltwoodite-Na	-9.41	5.18	14.58	Na.7K.3(H3O)(UO2)SiO4:H2O
Borax	0.00	12.04	12.04	Na2(B4O5(OH)4):8H2O
Boric_acid	-0.50	-0.66	-0.16	B(OH)3
Brucite	-4.31	11.97	16.28	Mg(OH)2
Brushite	-16.26	-9.71	6.55	CaHPO4:2H2O
Burkeite	-12.07	-2.58	9.49	Na6CO3(SO4)2
C	-71.88	-93.73	-21.85	C
C(g)	-189.50	-93.73	95.77	C
Ca	-124.88	-28.05	96.83	Ca
Ca(g)	-150.12	-28.05	122.07	Ca
Ca-Al_Pyroxene	-11.99	23.91	35.90	CaAl2SiO6
Ca2Al2O5:8H2O	-18.53	41.04	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-22.36	3.93	26.29	Ca2Cl2(OH)2:H2O
Ca2V2O7	-0.48	16.71	17.18	Ca2V2O7
Ca3(AsO4)2	-53.49	-35.69	17.80	Ca3(AsO4)2
Ca3Al2O6	-58.79	54.25	113.03	Ca3Al2O6
Ca3V2O8	-8.71	29.86	38.57	Ca3V2O8
Ca4Al2Fe2O10	-61.79	104.73	166.52	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-39.94	67.32	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-36.40	67.28	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-38.18	30.15	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-18.97	27.94	46.91	CaAl2O4
CaAl2O4:10H2O	-10.12	27.88	37.99	CaAl2O4:10H2O
CaAl4O7	-25.87	42.73	68.59	CaAl4O7
Calcite	-0.00	1.82	1.82	CaCO3
Carnallite	-21.56	-17.29	4.27	KMgCl3:6H2O
Carnotite	4.07	4.59	0.51	K2(UO2)2(VO4)2
CaSeO3:2H2O	-14.93	-48.58	-33.65	CaSeO3:2H2O
CaSeO4	-4.28	-7.37	-3.09	CaSeO4
CaSO4:0.5H2O(beta)	-0.99	-4.52	-3.54	CaSO4:0.5H2O
CaUO4	-0.00	15.94	15.94	CaUO4
CaV2O6	-1.98	3.55	5.53	CaV2O6
Celadonite	0.25	7.56	7.31	KMgAlSi4O10(OH)2
CH4(g)	-145.41	-176.15	-30.74	CH4
Chalcedony	-0.27	-4.03	-3.76	SiO2
Chamosite-7A	-25.88	6.88	32.76	Fe2Al2SiO5(OH)4
Chloromagnesite	-32.20	-10.38	21.82	MgCl2
Chrysotile	-3.17	27.86	31.03	Mg3Si2O5(OH)4
Cl2(g)	-27.15	18.84	45.99	Cl2

```
     Claudetite      -112.83 -157.55  -44.73  As2O3
     Clinochlore-14A  -4.49   62.56   67.05  Mg5Al2Si3O10(OH)8
     Clinochlore-7A   -7.86   62.56   70.42  Mg5Al2Si3O10(OH)8
     Clinoptilolite-Ca  -2.69   -9.98   -7.29
Ca1.7335Al3.45Fe.017Si14.533O36:10.922H2O
     Clinoptilolite-dehy-Ca -38.27   -9.91   28.36
Ca1.7335Al3.45Fe.017Si14.533O36
     Clinoptilolite-dehy-K -42.19  -17.77   24.43
K3.467Al3.45Fe.017Si14.533O36
     Clinoptilolite-dehy-Na -35.47   -7.24   28.23
Na3.467Al3.45Fe.017Si14.533O36
     Clinoptilolite-dehy-NH4-254.96 -642.68 -387.72
(NH4)3.467Al3.45Fe.017Si14.533O36
     Clinoptilolite-hy-Ca  -2.69   -9.99   -7.29
Ca1.7335Al3.45Fe.017Si14.533O36:11.645H2O
     Clinoptilolite-hy-K  -6.58  -17.81  -11.23
K3.467Al3.45Fe.017Si14.533O36:7.499H2O
     Clinoptilolite-hy-Na   0.12   -7.31   -7.43
Na3.467Al3.45Fe.017Si14.533O36:10.877H2O
     Clinoptilolite-K  -6.61  -17.84  -11.23
K3.467Al3.45Fe.017Si14.533O36:10.922H2O
     Clinoptilolite-Na   0.12   -7.31   -7.42
Na3.467Al3.45Fe.017Si14.533O36:10.922H2O
     Clinoptilolite-NH4-219.39 -642.75 -423.36
(NH4)3.467Al3.45Fe.017Si14.533O36:10.922H2O
     Clinozoisite     -6.70   36.40   43.10  Ca2Al3Si3O12(OH)
     CO(g)           -48.21  -52.53   -4.32  CO
     CO2(g)           -3.50  -11.33   -7.83  CO2
     Coesite          -0.81   -4.03   -3.22  SiO2
     Coffinite       -25.33  -42.45  -17.12  USiO4
     Colemanite        0.87   22.39   21.51  Ca2B6O11:5H2O
     Cordierite_anhyd -18.68   33.39   52.07  Mg2Al4Si5O18
     Cordierite_hydr -16.20   33.38   49.59  Mg2Al4Si5O18:H2O
     Corundum         -3.50   14.79   18.29  Al2O3
     Cristobalite(alpha)  -0.55   -4.03   -3.48  SiO2
     Cristobalite(beta)  -0.99   -4.03   -3.03  SiO2
     Cronstedtite-7A -12.79   29.43   42.21  Fe2Fe2SiO5(OH)4
     Daphnite-14A    -59.09   -6.99   52.10  Fe5AlAlSi3O10(OH)8
     Daphnite-7A     -62.47   -6.99   55.48  Fe5AlAlSi3O10(OH)8
     Dawsonite        -0.93    3.41    4.34  NaAlCO3(OH)2
     Diaspore          0.24    7.39    7.15  AlHO2
     Dicalcium_silicate -14.85   22.28   37.13  Ca2SiO4
     Diopside         -3.81   17.07   20.89  CaMgSi2O6
     Dolomite         -0.00    2.47    2.47  CaMg(CO3)2
     Dolomite-dis     -1.54    2.47    4.01  CaMg(CO3)2
     Dolomite-ord      0.01    2.47    2.46  CaMg(CO3)2
     Downeyite       -25.92  -61.72  -35.81  SeO2
     Enstatite        -3.34    7.95   11.29  MgSiO3
     Epidote           1.88   47.67   45.79  Ca2FeAl2Si3O12OH
     Epidote-ord       1.89   47.67   45.78  FeCa2Al2(OH)(SiO4)3
     Epsomite         -3.78   -5.74   -1.96  MgSO4:7H2O
```

Ettringite	-21.98	40.49	62.46	Ca6Al2(SO4)3(OH)12:26H2O
F2(g)	-102.24	-3.53	98.71	F2
Fayalite	-26.96	-7.90	19.06	Fe2SiO4
Fe	-59.15	-43.13	16.02	Fe
Fe(OH)2	-15.83	-1.94	13.89	Fe(OH)2
Fe(OH)3	0.00	18.66	18.66	Fe(OH)3
Fe2(SO4)3	-44.77	-15.68	29.08	Fe2(SO4)3
FeF2	-44.24	-46.67	-2.42	FeF2
FeF3	-42.20	-48.44	-6.24	FeF3
FeO	-15.46	-1.93	13.52	FeO
Ferrite-Ca	2.96	50.49	47.53	CaFe2O4
Ferrite-Dicalcium	-19.19	63.64	82.84	Ca2Fe2O5
Ferrite-Mg	2.25	49.31	47.06	MgFe2O4
Ferrite-Zn	10.80	48.53	37.74	ZnFe2O4
Ferroselite	-152.57	-331.38	-178.81	FeSe2
Ferrosilite	-13.37	-5.96	7.41	FeSiO3
FeSO4	-22.21	-19.61	2.61	FeSO4
FeV2O4	-329.07	-93.94	235.14	FeV2O4
Fluorapatite	0.00	-25.16	-25.16	Ca5(PO4)3F
Fluorite	-21.51	-31.58	-10.07	CaF2
Forsterite	-7.88	19.93	27.81	Mg2SiO4
Foshagite	-25.28	40.52	65.80	Ca4Si3O9(OH)2:0.5H2O
Frankdicksonite	-31.32	-37.08	-5.76	BaF2
Gaylussite	-6.00	5.16	11.16	CaNa2(CO3)2:5H2O
Gehlenite	-19.16	37.06	56.22	Ca2Al2SiO7
Gibbsite	-0.36	7.38	7.74	Al(OH)3
Gismondine	-2.01	39.71	41.72	Ca2Al4Si4O16:9H2O
Glauberite	-2.03	-7.49	-5.47	Na2Ca(SO4)2
Goethite	5.12	18.66	13.55	FeOOH
Greenalite	-36.45	-13.87	22.58	Fe3Si2O5(OH)4
Grossular	-9.61	42.16	51.78	Ca3Al2(SiO4)3
Gypsum	-0.00	-4.53	-4.53	CaSO4:2H2O
Gyrolite	-8.60	14.21	22.80	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-41.21	-41.21	-0.00	H2
H2O(g)	-1.59	-0.01	1.59	H2O
H2S(g)	-140.78	-182.48	-41.70	H2S
Haiweeite	1.56	-5.48	-7.04	Ca(UO2)2(Si2O5)3:5H2O
Halite	-5.40	-3.83	1.56	NaCl
Hatrurite	-37.92	35.43	73.35	Ca3SiO5
Hausmannite	-11.61	49.68	61.29	Mn3O4
HCl(g)	-17.49	-11.18	6.30	HCl
Hedenbergite	-16.36	3.16	19.53	CaFe(SiO3)2
Hematite	11.22	37.33	26.11	Fe2O3
Hercynite	-15.95	12.85	28.80	FeAl2O4
Hexahydrite	-4.01	-5.73	-1.73	MgSO4:6H2O
HI(g)	-35.87	-137.80	-101.93	HI
Hillebrandite	-14.50	22.27	36.77	Ca2SiO3(OH)2:0.17H2O
Hopeite	-1.47	-12.13	-10.66	Zn3(PO4)2:4H2O
HTcO4	-21.37	-15.42	5.95	HTcO4
Huntite	-6.45	3.77	10.22	CaMg3(CO3)4
Hydroboracite	0.84	21.20	20.36	MgCaB6O11:6H2O

Hydromagnesite	-16.20	14.54	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.95	-9.21	11.75	CaCl2
Hydroxylapatite	0.43	-2.79	-3.22	Ca5(OH)(PO4)3
Hydrozincite	3.01	33.32	30.31	Zn5(OH)6(CO3)2
I2	-29.91	-234.40	-204.49	I2
I2(g)	-33.32	-234.40	-201.08	I2
Ice	-0.15	-0.01	0.14	H2O
Illite	-0.40	8.48	8.88	
K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2				
Jadeite	-1.62	6.69	8.31	NaAl(SiO3)2
Jarosite	-4.70	24.95	29.64	KFe3(SO4)2(OH)6
Jarosite-Na	-5.62	27.99	33.61	NaFe3(SO4)2(OH)6
K	-65.77	-16.29	49.48	K
K(g)	-76.37	-16.29	60.08	K
K-Feldspar	-0.00	-0.38	-0.38	KAlSi3O8
K2CO3:1.5H2O	-16.09	-2.72	13.38	K2CO3:1.5H2O
K2O	-75.41	8.62	84.04	K2O
K2Se	-121.74	-176.70	-54.97	K2Se
K2UO4	-22.47	11.40	33.87	K2UO4
K3H(SO4)2	-18.79	-22.41	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-61.22	-33.51	27.71	K8H4(CO3)6:3H2O
Kainite	-12.27	-12.58	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-26.91	-23.64	3.27	KAl(SO4)2
Kalicinite	-7.30	-7.02	0.28	KHCO3
Kalsilite	-3.17	7.68	10.85	KAlSiO4
Kaolinite	0.00	6.72	6.72	Al2Si2O5(OH)4
Karelianite	-56.53	-92.00	-35.47	V2O3
Katoite	-24.74	54.21	78.94	Ca3Al2H12O12
Kieserite	-5.43	-5.70	-0.27	MgSO4:H2O
KMgCl3	-38.50	-17.25	21.25	KMgCl3
KMgCl3:2H2O	-31.23	-17.27	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-9.97	0.29	10.26	KNaCO3:6H2O
KTcO4	-8.83	-11.10	-2.27	KTcO4
KUO2AsO4	-26.31	-30.48	-4.17	KUO2AsO4
Kyanite	-4.85	10.76	15.61	Al2SiO5
Lansfordite	-4.22	0.62	4.84	MgCO3:5H2O
Larnite	-16.14	22.28	38.42	Ca2SiO4
Laumontite	-1.71	11.80	13.51	CaAl2Si4O12:4H2O
Lawrencite	-33.35	-24.29	9.05	FeCl2
Lawsonite	-2.23	19.87	22.11	CaAl2Si2O7(OH)2:H2O
Leonite	-10.66	-14.77	-4.11	K2Mg(SO4)2:4H2O
Lime	-19.42	13.15	32.57	CaO
Magnesite	-1.62	0.65	2.27	MgCO3
Magnetite	-1.05	35.40	36.45	Fe3O4
Manganite	-1.98	23.42	25.41	MnO(OH)
Manganosite	-15.09	2.83	17.92	MnO
Margarite	-6.26	34.66	40.93	CaAl4Si2O10(OH)2
Maximum_Microcline	0.00	-0.38	-0.38	KAlSi3O8
Mayenite	-232.81	261.34	494.15	Ca12Al14O33
Melanterite	-17.25	-19.65	-2.40	FeSO4:7H2O
Mercallite	-11.93	-13.36	-1.44	KHSO4
Merwinite	-25.03	43.38	68.41	MgCa3(SiO4)2

```
     Mesolite            2.69   16.18   13.49
Na.676Ca.657Al1.99Si3.01O10:2.647H2O
     Mg               -108.75  -29.22   79.52  Mg
     Mg(g)            -128.47  -29.22   99.25  Mg
     Mg1.25SO4(OH)0.5:0.5H2O  -7.90   -2.71    5.20
Mg1.25SO4(OH)0.5:0.5H2O
     Mg1.5SO4(OH)       -8.92    0.29    9.21  Mg1.5SO4(OH)
     Mg2V2O7           -11.64   14.36   25.99  Mg2V2O7
     MgCl2:2H2O        -23.13  -10.40   12.73  MgCl2:2H2O
     MgCl2:4H2O        -17.71  -10.41    7.30  MgCl2:4H2O
     MgCl2:H2O         -26.46  -10.39   16.07  MgCl2:H2O
     MgOHCl            -15.10    0.79   15.89  MgOHCl
     MgSeO3            -22.40  -49.74  -27.34  MgSeO3
     MgSeO3:6H2O       -17.33  -49.78  -32.45  MgSeO3:6H2O
     MgSO4             -10.52   -5.69    4.83  MgSO4
     MgUO4              -8.23   14.76   22.99  MgUO4
     MgV2O6             -8.67    2.38   11.05  MgV2O6
     Minnesotaite      -35.75  -21.92   13.83  Fe3Si4O10(OH)2
     Mirabilite         -1.88   -3.04   -1.15  Na2SO4:10H2O
     Misenite          -78.16  -89.23  -11.08  K8H6(SO4)7
     Mn                -78.31  -38.37   39.94  Mn
     Mn(OH)2(am)       -12.49    2.82   15.31  Mn(OH)2
     Mn(OH)3            -8.50   23.42   31.92  Mn(OH)3
     Mn3(PO4)2         -38.04  -37.22    0.82  Mn3(PO4)2
     MnCl2:2H2O        -23.54  -19.55    4.00  MnCl2:2H2O
     MnCl2:4H2O        -22.31  -19.56    2.75  MnCl2:4H2O
     MnCl2:H2O         -25.08  -19.54    5.54  MnCl2:H2O
     MnHPO4             -7.08  -20.03  -12.95  MnHPO4
     MnO2(gamma)         0.93   44.03   43.10  MnO2
     MnSe             -105.55 -182.50  -76.95  MnSe
     MnSeO3            -22.61  -58.89  -36.29  MnSeO3
     MnSeO3:2H2O       -23.56  -58.91  -35.35  MnSeO3:2H2O
     MnSO4             -17.45  -14.84    2.61  MnSO4
     MnV2O6            -11.59   -6.77    4.82  MnV2O6
     Molysite          -41.36  -14.87   26.49  FeCl3
     Monohydrocalcite   -0.86    1.82    2.68  CaCO3:H2O
     Monticellite       -8.43   21.10   29.53  CaMgSiO4
     Montmor-Ca          0.01    2.35    2.34
Ca.165Mg.33Al1.67Si4O10(OH)2
     Montmor-K          -0.39    1.60    1.99
K.33Mg.33Al1.67Si4O10(OH)2
     Montmor-Mg         -0.08    2.16    2.23
Mg.495Al1.67Si4O10(OH)2
     Montmor-Na          0.28    2.61    2.33
Na.33Mg.33Al1.67Si4O10(OH)2
     Mordenite          -1.63   -6.99   -5.36
Ca.2895Na.361Al.94Si5.06O12:3.468H2O
     Mordenite-dehy    -16.74   -6.97    9.77
Ca.2895Na.361Al.94Si5.06O12
     Muscovite           0.95   14.40   13.45  KAl3Si3O10(OH)2
     N2(g)             -17.75 -228.24 -210.49  N2
     Na                -59.12  -13.25   45.87  Na
```

Na(g)	-72.61	-13.25	59.36	Na
Na2CO3	-7.80	3.37	11.16	Na2CO3
Na2CO3:7H2O	-6.62	3.32	9.94	Na2CO3:7H2O
Na2O	-52.72	14.70	67.42	Na2O
Na2Se	-116.21	-170.63	-54.42	Na2Se
Na2Se2	-163.89	-314.75	-150.86	Na2Se2
Na2SiO3	-11.53	10.67	22.20	Na2SiO3
Na2U2O7	-2.33	20.26	22.59	Na2U2O7
Na2UO4(alpha)	-12.54	17.48	30.02	Na2UO4
Na3H(SO4)2	-12.41	-13.30	-0.89	Na3H(SO4)2
Na3UO4	-50.53	4.23	54.76	Na3UO4
Na4Ca(SO4)3:2H2O	-4.59	-10.48	-5.89	Na4Ca(SO4)3:2H2O
Na4SiO4	-45.23	25.36	70.60	Na4SiO4
Na4UO2(CO3)3	-5.85	-1.81	4.04	Na4UO2(CO3)3
Na6Si2O7	-65.50	36.03	101.53	Na6Si2O7
NaFeO2	-6.89	26.02	32.90	NaFeO2
Nahcolite	-3.84	-3.98	-0.14	NaHCO3
NaTcO4	-9.59	-8.07	1.52	NaTcO4
Natrolite	-1.00	17.39	18.39	Na2Al2Si3O10:2H2O
Natron	-6.28	3.30	9.59	Na2CO3:10H2O
Natrosilite	-11.42	6.64	18.07	Na2Si2O5
NaUO3	-17.32	-10.47	6.85	NaUO3
Nepheline	-3.04	10.71	13.75	NaAlSiO4
Nesquehonite	-4.66	0.63	5.29	MgCO3:3H2O
NH3(g)	-67.81	-175.93	-108.13	NH3
NH4HSe	-163.03	-361.26	-198.23	NH4HSe
Ningyoite	-32.12	-70.98	-38.86	CaUP2O8:2H2O
Niter	-6.58	-6.81	-0.22	KNO3
Nitrobarite	-12.08	-14.57	-2.49	Ba(NO3)2
NO(g)	-24.39	-72.92	-48.53	NO
NO2(g)	-18.57	-31.72	-13.15	NO2
Nontronite-Ca	12.85	27.16	14.31	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	11.64	24.98	13.35	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	12.38	26.41	14.02	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	12.69	26.96	14.27	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	13.05	27.41	14.36	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-0.70	82.40	83.10	O2
Okenite	-5.23	5.09	10.31	CaSi2O4(OH)2:H2O
Orpiment	-499.45	-704.98	-205.54	As2S3
Oxychloride-Mg	-13.09	12.74	25.83	Mg2Cl(OH)3:4H2O
P	-150.41	-125.86	24.56	P
Paragonite	0.06	17.44	17.38	NaAl3Si3O10(OH)2
Pargasite	-22.13	79.57	101.70	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrite	-4.34	-5.73	-1.39	MgSO4:5H2O
Periclase	-9.35	11.98	21.33	MgO
Phlogopite	-1.75	35.55	37.30	KAlMg3Si3O10(OH)2
Picromerite	-10.34	-14.78	-4.44	K2Mg(SO4)2:6H2O

Pirssonite	-6.14	5.18	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-9.48	-23.79	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-9.40	13.15	22.55	Ca(OH)2
Prehnite	-3.79	29.00	32.79	Ca2Al2Si3O10(OH)2
Pseudowollastonite	-4.84	9.13	13.96	CaSiO3
Pu	-174.14	-108.33	65.81	Pu
Pu(HPO4)2	-25.31	-71.64	-46.33	Pu(HPO4)2
Pu(OH)3	-33.43	-46.54	-13.11	Pu(OH)3
Pu(OH)4	-8.14	-25.94	-17.81	Pu(OH)4
Pu2O3	-70.07	-93.06	-22.98	Pu2O3
PuF3	-67.83	-113.63	-45.80	PuF3
PuF4	-83.55	-115.40	-31.85	PuF4
PuO2	0.00	-25.93	-25.93	PuO2
PuO2(OH)2	-4.59	15.27	19.86	PuO2(OH)2
PuO2HPO4	-11.24	-7.58	3.66	PuO2HPO4
PuO2OH(am)	-10.79	-5.33	5.46	PuO2OH
Pyrite	-242.00	-325.69	-83.69	FeS2
Pyrolusite	2.47	44.03	41.56	MnO2
Pyrophyllite	-1.62	-1.33	0.29	Al2Si4O10(OH)2
Pyrrhotite	-146.96	-184.41	-37.45	FeS
Quartz	0.00	-4.03	-4.03	SiO2
Rankinite	-20.42	31.40	51.82	Ca3Si2O7
Realgar	-200.74	-281.85	-81.11	AsS
Rhodochrosite	-8.28	-8.50	-0.22	MnCO3
Rhodonite	-10.89	-1.20	9.69	MnSiO3
Ripidolite-14A	-26.04	34.74	60.78	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	-29.42	34.74	64.16	Mg3Fe2Al2Si3O10(OH)8
Rutherfordine	-4.43	-8.55	-4.12	UO2CO3
S	-105.46	-141.28	-35.82	S
S2(g)	-224.80	-282.55	-57.75	S2
Saleeite	-8.69	-28.16	-19.48	Mg(UO2)2(PO4)2
Sanbornite	-9.80	-0.40	9.41	BaSi2O5
Sanidine_high	-1.20	-0.38	0.82	KAlSi3O8
Saponite-Ca	-0.39	25.75	26.14	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	-1.60	23.58	25.18	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	-0.85	25.01	25.86	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	-0.54	25.56	26.10	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	-0.19	26.01	26.20	Na.33Mg3Al.33Si3.67O10(OH)2
Scacchite	-28.27	-19.53	8.74	MnCl2
Schoepite	-2.07	2.77	4.83	UO3:2H2O
Schoepite-dehy(.393)	-3.95	2.78	6.72	UO3:.393H2O
Schoepite-dehy(.648)	-3.43	2.78	6.21	UO3:.648H2O
Schoepite-dehy(.85)	-2.32	2.78	5.10	UO3:.85H2O
Schoepite-dehy(.9)	-2.24	2.78	5.02	UO3:.9H2O
Schoepite-dehy(1.0)	-2.33	2.78	5.10	UO3:H2O
Scolecite	0.09	15.84	15.75	CaAl2Si3O10:3H2O
Se	-55.21	-144.12	-88.92	Se

Se2O5	-62.72	-82.24	-19.53	Se2O5
SeCl4	-91.76	-106.44	-14.68	SeCl4
Sellaite	-23.31	-32.76	-9.44	MgF2
SeO3	-39.68	-20.52	19.16	SeO3
Sepiolite	-6.52	23.70	30.22	Mg4Si6O15(OH)2:6H2O
Shcherbinaite	-8.15	-9.60	-1.45	V2O5
Si	-149.30	-86.43	62.87	Si
Si(g)	-220.37	-86.43	133.94	Si
Siderite	-13.04	-13.26	-0.22	FeCO3
SiF4(g)	-78.26	-93.50	-15.24	SiF4
Sillimanite	-5.49	10.76	16.24	Al2SiO5
SiO2(am)	-1.29	-4.03	-2.74	SiO2
Sklodowskite	-4.35	9.44	13.79	
Mg(H3O)2(UO2)2(SiO4)2:4H2O				
Smectite-high-Fe-Mg	-6.27	13.60	19.88	
Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12				
Smectite-low-Fe-Mg	-3.41	9.56	12.98	
Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12				
Smithsonite	-0.57	-0.13	0.44	ZnCO3
SO2(g)	-53.56	-58.87	-5.32	SO2
Soddyite	1.13	1.52	0.39	(UO2)2SiO4:2H2O
Sphalerite	-126.10	-171.28	-45.18	ZnS
Spinel	-10.84	26.76	37.61	Al2MgO4
Starkeyite	-4.72	-5.72	-1.00	MgSO4:4H2O
Stilbite	2.22	3.03	0.81	
Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O				
Stilleite	-83.89	-174.13	-90.24	ZnSe
Strengite	-5.82	-4.20	1.63	FePO4:2H2O
Sylvite	-7.70	-6.87	0.83	KCl
Syngenite	-5.97	-13.57	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-47.19	-30.05	17.14	Mg2CaCl6:12H2O
Talc	-1.17	19.81	20.99	Mg3Si4O10(OH)2
Tb	-158.69	-41.80	116.89	Tb
Tb(OH)3	4.31	19.99	15.69	Tb(OH)3
Tb(OH)3(am)	1.21	19.99	18.79	Tb(OH)3
Tb2(CO3)3	9.24	6.02	-3.21	Tb2(CO3)3
Tb2O3	-7.09	40.01	47.10	Tb2O3
TbF3:.5H2O	-30.40	-47.10	-16.70	TbF3:.5H2O
TbPO4:10H2O	9.07	-2.91	-11.98	TbPO4:10H2O
Tc	-102.70	-159.62	-56.92	Tc
Tc(OH)2	-63.82	-118.42	-54.61	Tc(OH)2
Tc(OH)3	-50.20	-97.83	-47.62	Tc(OH)3
Tc2O7	-43.93	-30.83	13.10	Tc2O7
Tc2O7(g)	-52.18	-30.83	21.35	Tc2O7
Tc2S7	-841.94	-1308.17	-466.23	Tc2S7
Tc3O4	-158.18	-314.05	-155.87	Tc3O4
Tc4O7	-181.31	-350.07	-168.76	Tc4O7
TcO2:2H2O(am)	-40.01	-77.23	-37.22	TcO2:2H2O
TcO3	-23.19	-36.01	-12.83	TcO3
TcOH	-82.54	-139.02	-56.48	TcOH
TcS2	-275.79	-442.17	-166.38	TcS2
TcS3	-373.14	-583.45	-210.30	TcS3

Tephroite	-21.40	1.63	23.02	Mn2SiO4
Thenardite	-2.62	-2.98	-0.36	Na2SO4
Thermonatrite	-7.58	3.36	10.94	Na2CO3:H2O
Tobermorite-11A	-23.82	41.57	65.39	Ca5Si6H11O22.5
Tobermorite-14A	-22.08	41.53	63.61	Ca5Si6H21O27.5
Tobermorite-9A	-27.27	41.58	68.86	Ca5Si6H6O20
Todorokite	-0.29	225.78	226.07	Mn7O12:3H2O
Tremolite	-6.96	53.96	60.93	Ca2Mg5Si8O22(OH)2
Tridymite	-0.19	-4.03	-3.84	SiO2
Troilite	-146.86	-184.41	-37.55	FeS
Trona-K	-18.29	-6.70	11.59	K2NaH(CO3)2:2H2O
Tyuyamunite	5.60	9.12	3.52	Ca(UO2)2(VO4)2
U	-204.60	-120.82	83.77	U
U(CO3)2	-59.55	-61.08	-1.53	U(CO3)2
U(g)	-290.15	-120.82	169.33	U
U(HPO4)2:4H2O	-42.18	-84.15	-41.98	U(HPO4)2:4H2O
U(OH)2SO4	-43.97	-56.10	-12.12	U(OH)2SO4
U(SO3)2	-117.59	-156.17	-38.58	U(SO3)2
U(SO4)2	-53.18	-73.76	-20.58	U(SO4)2
U(SO4)2:4H2O	-53.19	-73.79	-20.60	U(SO4)2:4H2O
U(SO4)2:8H2O	-52.20	-73.81	-21.62	U(SO4)2:8H2O
U2C3	-591.67	-522.84	68.84	U2C3
U2Cl10(g)	-227.08	-147.44	79.64	U2Cl10
U2Cl8(g)	-230.46	-166.28	64.17	U2Cl8
U2F10(g)	-243.88	-259.31	-15.44	U2F10
U2F9	-201.36	-257.55	-56.19	U2F9
U2O2Cl5	-120.80	-112.14	8.66	U2O2Cl5
U2O3F6	-126.11	-128.64	-2.53	U2O3F6
U2S3	-571.43	-665.47	-94.04	U2S3
U2Se3	-448.59	-674.02	-225.43	U2Se3
U3As4	-911.92	-924.78	-12.86	U3As4
U3O5F8	-167.71	-170.59	-2.88	U3O5F8
U3P4	-1070.70	-865.89	204.81	U3P4
U3S5	-891.49	-1068.85	-177.36	U3S5
U3Se4	-661.56	-938.96	-277.41	U3Se4
U3Se5	-691.94	-1083.09	-391.15	U3Se5
U4F17	-379.61	-513.32	-133.72	U4F17
U5O12Cl	-74.08	-100.27	-26.20	U5O12Cl
UAs	-269.22	-261.40	7.82	UAs
UAs2	-372.91	-401.98	-29.06	UAs2
UC	-259.15	-214.55	44.60	UC
UC1.94(alpha)	-328.75	-302.66	26.09	UC1.94
UCl(g)	-245.68	-111.40	134.28	UCl
UCl2(g)	-199.73	-101.98	97.75	UCl2
UCl2F2	-92.88	-105.52	-12.64	UCl2F2
UCl2I2	-134.96	-336.38	-201.41	UCl2I2
UCl3	-105.83	-92.56	13.27	UCl3
UCl3(g)	-151.44	-92.56	58.88	UCl3
UCl3F	-95.52	-94.33	1.19	UCl3F
UCl3I	-114.91	-209.76	-94.84	UCl3I
UCl4	-96.01	-83.14	12.87	UCl4
UCl4(g)	-120.44	-83.14	37.30	UCl4

UCl5	-109.47	-73.72	35.75	UCl5
UCl5(g)	-126.69	-73.72	52.97	UCl5
UCl6	-121.80	-64.30	57.50	UCl6
UCl6(g)	-127.67	-64.30	63.37	UCl6
UClF3	-90.07	-116.70	-26.64	UClF3
UClI3	-155.20	-462.99	-307.80	UClI3
UF(g)	-241.34	-122.59	118.76	UF
UF2(g)	-210.68	-124.36	86.32	UF2
UF3	-106.96	-126.12	-19.17	UF3
UF3(g)	-173.61	-126.12	47.49	UF3
UF4	-89.58	-127.89	-38.31	UF4
UF4(g)	-133.37	-127.89	5.48	UF4
UF4:2.5H2O	-85.41	-127.91	-42.49	UF4:2.5H2O
UF5(alpha)	-115.23	-129.66	-14.42	UF5
UF5(beta)	-114.91	-129.66	-14.75	UF5
UF5(g)	-134.46	-129.66	4.80	UF5
UF6	-148.73	-131.42	17.31	UF6
UF6(g)	-149.57	-131.42	18.15	UF6
UH3(beta)	-253.71	-182.63	71.07	UH3
UI(g)	-270.00	-238.02	31.98	UI
UI2(g)	-241.06	-355.22	-114.15	UI2
UI3	-167.71	-472.41	-304.71	UI3
UI3(g)	-214.31	-472.41	-258.11	UI3
UI4	-174.52	-589.61	-415.09	UI4
UI4(g)	-199.53	-589.61	-390.09	UI4
UN	-167.02	-234.94	-67.93	UN
UN1.59(alpha)	-159.46	-302.27	-142.81	UN1.59
UN1.73(alpha)	-157.98	-318.25	-160.27	UN1.73
UO(g)	-205.27	-79.62	125.65	UO
UO2(am)	-29.48	-38.42	-8.94	UO2
UO2(AsO3)2	-79.28	-72.37	6.91	UO2(AsO3)2
UO2(g)	-121.02	-38.42	82.60	UO2
UO2(IO3)2	-18.31	-25.61	-7.29	UO2(IO3)2
UO2(NO3)2	-31.40	-19.45	11.95	UO2(NO3)2
UO2(NO3)2:2H2O	-24.37	-19.46	4.91	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-23.15	-19.47	3.68	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-21.78	-19.49	2.29	UO2(NO3)2:6H2O
UO2(NO3)2:H2O	-27.96	-19.46	8.50	UO2(NO3)2:H2O
UO2(OH)2(beta)	-2.17	2.78	4.95	UO2(OH)2
UO2(PO3)2	-26.58	-42.92	-16.34	UO2(PO3)2
UO2.25	-18.02	-28.12	-10.10	UO2.25
UO2.25(beta)	-18.09	-28.12	-10.02	UO2.25
UO2.3333(beta)	-32.22	-49.37	-17.15	(UO2.3333)2
UO2.6667	-17.53	-21.90	-4.37	(UO2.6667)2
UO2Cl	-26.98	-29.00	-2.02	UO2Cl
UO2Cl2	-31.69	-19.58	12.11	UO2Cl2
UO2Cl2(g)	-67.51	-19.58	47.93	UO2Cl2
UO2Cl2:3H2O	-25.21	-19.60	5.61	UO2Cl2:3H2O
UO2Cl2:H2O	-27.87	-19.59	8.28	UO2Cl2:H2O
UO2ClOH:2H2O	-10.72	-8.41	2.30	UO2ClOH:2H2O
UO2CO3	-4.42	-8.55	-4.13	UO2CO3
UO2F2	-34.69	-41.95	-7.27	UO2F2

UO2F2(g)	-76.58	-41.95	34.63	UO2F2
UO2F2:3H2O	-34.59	-41.97	-7.38	UO2F2:3H2O
UO2FOH	-17.74	-19.59	-1.85	UO2FOH
UO2FOH:2H2O	-16.93	-19.60	-2.67	UO2FOH:2H2O
UO2FOH:H2O	-17.31	-19.60	-2.29	UO2FOH:H2O
UO2HPO4	-7.39	-20.07	-12.68	UO2HPO4
UO2HPO4:4H2O	-7.07	-20.10	-13.03	UO2HPO4:4H2O
UO2SO3	-43.72	-56.09	-12.37	UO2SO3
UO2SO4	-16.82	-14.89	1.93	UO2SO4
UO2SO4:2.5H2O	-13.40	-14.91	-1.50	UO2SO4:2.5H2O
UO2SO4:3.5H2O	-13.42	-14.91	-1.49	UO2SO4:3.5H2O
UO2SO4:3H2O	-13.50	-14.91	-1.41	UO2SO4:3H2O
UO2SO4:H2O	-8.83	-14.90	-6.07	UO2SO4:H2O
UO3(alpha)	-5.86	2.78	8.64	UO3
UO3(beta)	-5.53	2.78	8.31	UO3
UO3(g)	-68.17	2.78	70.95	UO3
UO3(gamma)	-4.93	2.78	7.71	UO3
UO3:.9H2O(alpha)	-2.24	2.78	5.02	UO3:.9H2O
UO3:2H2O	-2.07	2.77	4.84	UO3:2H2O
UOCl	-80.87	-70.20	10.67	UOCl
UOCl2	-57.15	-60.78	-3.63	UOCl2
UOCl3	-62.46	-51.36	11.10	UOCl3
UOF2	-55.95	-83.15	-27.20	UOF2
UOF2:H2O	-55.40	-83.16	-27.76	UOF2:H2O
UOF4	-91.25	-86.69	4.56	UOF4
UOF4(g)	-110.90	-86.69	24.21	UOF4
UOFOH	-42.81	-60.79	-17.98	UOFOH
UOFOH:.5H2O	-42.36	-60.79	-18.43	UOFOH:.5H2O
UP	-308.44	-246.68	61.76	UP
UP2	-453.82	-372.53	81.29	UP2
UP2O7	-42.00	-84.12	-42.12	UP2O7
UP2O7:20H2O	-46.57	-84.25	-37.68	UP2O7:20H2O
UPO5	-19.58	-40.67	-21.09	UPO5
Uraninite	-24.54	-38.42	-13.88	UO2
Uranium-selenide	-211.29	-264.95	-53.65	USe
Uranocircite	-12.66	-32.48	-19.82	Ba(UO2)2(PO4)2
Uranophane	-6.63	10.65	17.29	Ca(UO2)2(SiO3)2(OH)2
US	-253.83	-262.10	-8.27	US
US1.9	-315.71	-389.25	-73.53	US1.9
US2	-324.55	-403.37	-78.83	US2
US3	-426.84	-544.65	-117.81	US3
USe2(alpha)	-240.19	-409.07	-168.88	USe2
USe2(beta)	-240.04	-409.07	-169.03	USe2
USe3	-291.14	-553.20	-262.05	USe3
V	-127.54	-107.80	19.74	V
V2O4	-25.53	-50.80	-25.27	V2O4
V3O5	-68.50	-117.40	-48.91	V3O5
V4O7	-82.35	-142.80	-60.45	V4O7
Vivianite	-46.83	-51.55	-4.72	Fe3(PO4)2:8H2O
Wairakite	-6.10	11.82	17.92	CaAl2Si4O10(OH)4
Weeksite	-25.38	-10.01	15.38	K2(UO2)2(Si2O5)3:4H2O
Whitlockite	-1.92	-6.24	-4.32	Ca3(PO4)2

Witherite	-0.65	-3.67	-3.02	BaCO3
Wollastonite	-4.60	9.13	13.72	CaSiO3
Wurtzite	-128.40	-171.28	-42.88	ZnS
Wustite	-13.43	0.35	13.78	Fe.947O
Xonotlite	-36.99	54.75	91.74	Ca6Si6O17(OH)2
Yb	-154.73	-42.60	112.13	Yb
Yb(OH)3	4.51	19.19	14.69	Yb(OH)3
Yb(OH)3(am)	0.21	19.19	18.99	Yb(OH)3
Yb2(CO3)3	6.73	4.42	-2.31	Yb2(CO3)3
Yb2O3	-9.39	38.41	47.80	Yb2O3
YbF3:.5H2O	-31.90	-47.90	-16.00	YbF3:.5H2O
YbPO4:10H2O	8.07	-3.71	-11.78	YbPO4:10H2O
Zincite	-0.00	11.20	11.20	ZnO
Zn	-55.79	-30.00	25.79	Zn
Zn(BO2)2	1.59	9.90	8.31	Zn(BO2)2
Zn(ClO4)2:6H2O	-62.65	318.41	381.06	Zn(ClO4)2:6H2O
Zn(g)	-72.41	-30.00	42.41	Zn
Zn(IO3)2	-11.87	-17.19	-5.32	Zn(IO3)2
Zn(NO3)2:6H2O	-14.47	-11.07	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-0.74	11.19	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-0.47	11.19	11.66	Zn(OH)2
Zn(OH)2(gamma)	-0.69	11.19	11.88	Zn(OH)2
Zn2(OH)3Cl	-4.08	11.21	15.29	Zn2(OH)3Cl
Zn2SiO4	4.53	18.37	13.84	Zn2SiO4
Zn2SO4(OH)2	-2.86	4.72	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-50.86	-41.55	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-20.84	-1.75	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-8.93	33.74	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.24	-11.16	7.08	ZnCl2
ZnCl2(NH3)2	-136.17	-363.02	-226.85	ZnCl2(NH3)2
ZnCl2(NH3)4	-268.49	-714.89	-446.40	ZnCl2(NH3)4
ZnCl2(NH3)6	-402.47	-1066.75	-664.28	ZnCl2(NH3)6
ZnCO3:H2O	-0.28	-0.14	0.14	ZnCO3:H2O
ZnF2	-33.04	-33.54	-0.49	ZnF2
ZnI2	-49.13	-264.40	-215.27	ZnI2
ZnSeO3:H2O	-14.76	-50.53	-35.77	ZnSeO3:H2O
ZnSO4	-10.01	-6.47	3.53	ZnSO4
ZnSO4:6H2O	-4.81	-6.51	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.64	-6.52	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-5.93	-6.48	-0.55	ZnSO4:H2O
Zoisite	-6.74	36.40	43.14	Ca2Al3(SiO4)3OH

End of simulation.

Reading input data for simulation 3.

End of run.

B-3 Sensitivity: Assume 20,000 gal/week of applied water instead of 10,000 gal/week. Input file.

```
TITLE Rerun previous assemblage with a new mixing ratio
SOLUTION 1 Average Rainfall Composition
        units   mg/L
        pH      5.6
        pe      8.451
        temp    25.0
        redox   O(0)/O(-2)
        O(0)            1.0     O2(g) -0.7
Na    2
K     0.27
Ca    0.13
Mg    0.27
C     0.36
Cl    3.8
S(6)  0.62
SOLUTION 2 INEEL Water Quality (CPP-1, 6/6/91)
units  mg/L
pH    8
pe     8.4
redox   O(0)/O(-2)
        O(0)            1.0     O2(g) -0.7
C     194
Ca    54
Mg    14
Na    7.9
K     2.5
Cl    18
S(6)  22
MIX 1 Mixing Solutions 1 and 2
1   0.74
2   0.26
SAVE SOLUTION  3
END
USE SOLUTION  3
REACTION
NaCN  2.16e-04
NaI   9.49e-07
1.0
EQUILIBRIUM_PHASES 1
Calcite     0.0  6.1
Illite      0.0   4.1
Kaolinite   0.0  0.0
Quartz      0.0  106.5
Gypsum      0.0   0.0013
Albite      0.0  14.4
K-Feldspar  0.0  7.8
Fluorapatite  0.0  0.017
```

```
Dolomite  0.0   Enstatite  21.7
Yb2O3  0.0  0.0094
Fe(OH)3  0.0  2.89
Pyrite  0.0  0.17
Zincite  0.0  Sphalerite  0.05
Birnessite  0.0  0.008
Barite  0.0  0.022
Borax  0.0  0.07
PuO2   0.0  8.76e-09
CaUO4  0.0  0.000417
Ca2V2O7  0.0  0.0035
Tb2O3    0.0  0.03
TcO2:2H2O(am)   0.0  5.72e-08
Ca3(AsO4)2  0.0  0.0006
Niter  0.0  0.001
Halite    0.0  0.0009
CaSeO4    0.0  1.8e-04
O2(g)   -0.7   1.0
CO2(g)    -3.5   1.0
END
```

B-4 Sensitivity: Assume 20,000 gal/week of applied water instead of 10,000 gal/week. Output file.

```
Input file: C:\Documents\INEEL\pqe2\EDF274_update2.pqi
  Output file: C:\Documents\INEEL\pqe2\EDF274_update2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive\llnl.dat

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

      LLNL_AQUEOUS_MODEL_PARAMETERS
      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\USGS\Phreeqc Interactive\llnl.dat
      TITLE Rerun previous assemblage with a new mixing ratio
      SOLUTION 1 Average Rainfall Composition
              units   mg/L
              pH      5.6
              pe      8.451
              temp    25.0
              redox   O(0)/O(-2)
              O(0)            1.0     O2(g) -0.7
      Na    2
      K     0.27
      Ca    0.13
      Mg    0.27
      C     0.36
      Cl    3.8
      S(6)  0.62
      SOLUTION 2 INEEL Water Quality (CPP-1, 6/6/91)
      units  mg/L
      pH    8
      pe     8.4
      redox   O(0)/O(-2)
              O(0)            1.0     O2(g) -0.7
      C     194
      Ca    54
      Mg    14
```

```
     Na    7.9
     K     2.5
     Cl    18
     S(6)  22
     MIX 1 Mixing Solutions 1 and 2
     1   0.74
     2   0.26
     SAVE SOLUTION  3
     END
-----
TITLE
-----

 Rerun previous assemblage with a new mixing ratio

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

Initial solution 1.   Average Rainfall Composition

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

     Elements           Molality       Moles

     C                5.902e-006  5.902e-006
     Ca               3.244e-006  3.244e-006
     Cl               1.072e-004  1.072e-004
     K                6.906e-006  6.906e-006
     Mg               1.111e-005  1.111e-005
     Na               8.700e-005  8.700e-005
     O(0)             5.113e-004  5.113e-004  Equilibrium with
O2(g)
     S(6)             6.456e-006  6.456e-006

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

                                        pH  =   5.600
                                        pe  =   8.451
                           Activity of water  =   1.000
                              Ionic strength  =  1.438e-004
                        Mass of water (kg)    =  1.000e+000
                  Total alkalinity (eq/kg)    = -1.669e-006
                        Total CO2 (mol/kg)    =  5.902e-006
                      Temperature (deg C)     =  25.000
                   Electrical balance (eq)    =  4.179e-006
 Percent error, 100*(Cat-|An|)/(Cat+|An|)     =   1.70
                                 Iterations    =   4
                                    Total H    = 1.110507e+002
                                    Total O    = 5.552587e+001
```

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	15.0007	0.8874

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.546e-006	2.512e-006	-5.594	-5.600	-0.006
OH-	3.889e-009	3.836e-009	-8.410	-8.416	-0.006
H2O	5.553e+001	1.000e+000	-0.000	-0.000	0.000
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-266.969	-266.969	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-239.283	-239.283	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-148.571	-148.571	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-51.542	-51.542	0.000
C(4)	5.902e-006				
CO2	5.027e-006	5.027e-006	-5.299	-5.299	0.000
HCO3-	8.748e-007	8.627e-007	-6.058	-6.064	-0.006
MgHCO3+	1.067e-010	1.052e-010	-9.972	-9.978	-0.006
NaHCO3	1.059e-010	1.059e-010	-9.975	-9.975	0.000
CaHCO3+	3.179e-011	3.136e-011	-10.498	-10.504	-0.006
CO3-2	1.611e-011	1.524e-011	-10.793	-10.817	-0.024
MgCO3	1.692e-013	1.692e-013	-12.771	-12.771	0.000
CaCO3	1.083e-013	1.083e-013	-12.965	-12.965	0.000

```
     NaCO3-          4.638e-015  4.574e-015   -14.334   -14.340
-0.006
Ca              3.244e-006
     Ca+2            3.241e-006  3.067e-006    -5.489    -5.513
-0.024
     CaSO4           2.725e-009  2.725e-009    -8.565    -8.565
0.000
     CaCl+           6.967e-011  6.871e-011   -10.157   -10.163
-0.006
     CaHCO3+         3.179e-011  3.136e-011   -10.498   -10.504
-0.006
     CaOH+           1.749e-013  1.725e-013   -12.757   -12.763
-0.006
     CaCO3           1.083e-013  1.083e-013   -12.965   -12.965
0.000
     CaCl2           8.542e-015  8.542e-015   -14.068   -14.068
0.000
Cl(-1)          1.072e-004
     Cl-             1.072e-004  1.057e-004    -3.970    -3.976
-0.006
     NaCl            1.594e-009  1.594e-009    -8.798    -8.798
0.000
     MgCl+           8.786e-010  8.665e-010    -9.056    -9.062
-0.006
     CaCl+           6.967e-011  6.871e-011   -10.157   -10.163
-0.006
     HCl             5.963e-011  5.963e-011   -10.225   -10.225
0.000
     KCl             2.417e-011  2.417e-011   -10.617   -10.617
0.000
     CaCl2           8.542e-015  8.542e-015   -14.068   -14.068
0.000
Cl(1)           1.233e-019
     HClO            1.219e-019  1.219e-019   -18.914   -18.914
0.000
     ClO-            1.327e-021  1.309e-021   -20.877   -20.883
-0.006
Cl(3)           2.103e-031
     ClO2-           2.095e-031  2.066e-031   -30.679   -30.685
-0.006
     HClO2           7.674e-034  7.674e-034   -33.115   -33.115
0.000
Cl(5)           2.354e-027
     ClO3-           2.354e-027  2.321e-027   -26.628   -26.634
-0.006
Cl(7)           1.320e-027
     ClO4-           1.320e-027  1.301e-027   -26.880   -26.886
-0.006
H(0)            0.000e+000
     H2              0.000e+000  0.000e+000   -44.302   -44.302
0.000
K               6.906e-006
```

```
     K+                  6.905e-006  6.810e-006    -5.161    -5.167
-0.006
     KSO4-               3.390e-010  3.343e-010    -9.470    -9.476
-0.006
     KCl                 2.417e-011  2.417e-011   -10.617   -10.617
0.000
     KOH                 9.400e-015  9.400e-015   -14.027   -14.027
0.000
     KHSO4               7.410e-016  7.410e-016   -15.130   -15.130
0.000
Mg                 1.111e-005
     Mg+2                1.109e-005  1.050e-005    -4.955    -4.979
-0.024
     MgSO4               1.706e-008  1.706e-008    -7.768    -7.768
0.000
     MgCl+               8.786e-010  8.665e-010    -9.056    -9.062
-0.006
     MgHCO3+             1.067e-010  1.052e-010    -9.972    -9.978
-0.006
     MgCO3               1.692e-013  1.692e-013   -12.771   -12.771
0.000
     Mg4(OH)4+4          6.773e-038  5.429e-038   -37.169   -37.265
-0.096
Na                 8.700e-005
     Na+                 8.699e-005  8.579e-005    -4.061    -4.067
-0.006
     NaSO4-              3.496e-009  3.448e-009    -8.456    -8.462
-0.006
     NaCl                1.594e-009  1.594e-009    -8.798    -8.798
0.000
     NaHCO3              1.059e-010  1.059e-010    -9.975    -9.975
0.000
     NaOH                5.677e-014  5.677e-014   -13.246   -13.246
0.000
     NaCO3-              4.638e-015  4.574e-015   -14.334   -14.340
-0.006
O(0)               5.113e-004
     O2                  2.556e-004  2.556e-004    -3.592    -3.592
0.000
S(6)               6.456e-006
     SO4-2               6.430e-006  6.083e-006    -5.192    -5.216
-0.024
     MgSO4               1.706e-008  1.706e-008    -7.768    -7.768
0.000
     NaSO4-              3.496e-009  3.448e-009    -8.456    -8.462
-0.006
     CaSO4               2.725e-009  2.725e-009    -8.565    -8.565
0.000
     HSO4-               1.565e-009  1.543e-009    -8.805    -8.812
-0.006
     KSO4-               3.390e-010  3.343e-010    -9.470    -9.476
-0.006
```

```
     KHSO4              7.410e-016  7.410e-016   -15.130   -15.130
0.000
     H2SO4              3.658e-018  3.658e-018   -17.437   -17.437
0.000

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

     Phase                SI log IAP  log KT

     Anhydrite         -6.38  -10.73   -4.35  CaSO4
     Antarcticite     -17.56  -13.47    4.09  CaCl2:6H2O
     Aphthitalite     -26.11  -30.00   -3.89  NaK3(SO4)2
     Aragonite         -7.95   -5.98    1.97  CaCO3
     Arcanite         -13.71  -15.55   -1.84  K2SO4
     Artinite         -18.85    0.78   19.63  Mg2CO3(OH)2:3H2O
     Bassanite         -7.02  -10.73   -3.71  CaSO4:0.5H2O
     Bischofite       -17.32  -12.93    4.39  MgCl2:6H2O
     Bloedite         -21.07  -23.54   -2.48  Na2Mg(SO4)2:4H2O
     Brucite          -10.06    6.22   16.28  Mg(OH)2
     Burkeite         -44.78  -35.30    9.49  Na6CO3(SO4)2
     C                -72.22   -8.07   64.15  C
     C(g)            -189.84   -8.07  181.77  C
     Ca              -132.35    7.48  139.83  Ca
     Ca(g)           -157.59    7.48  165.07  Ca
     Ca2Cl2(OH)2:H2O -34.07   -7.78   26.29  Ca2Cl2(OH)2:H2O
     Ca4Cl2(OH)6:13H2O -64.73    3.59   68.33  Ca4Cl2(OH)6:13H2O
     Calcite           -7.80   -5.98    1.82  CaCO3
     Carnallite       -26.35  -22.07    4.27  KMgCl3:6H2O
     CaSO4:0.5H2O(beta)  -7.19  -10.73   -3.54  CaSO4:0.5H2O
     CH4(g)          -145.73   -4.48  141.25  CH4
     Chloromagnesite -34.75  -12.93   21.82  MgCl2
     Cl2(g)           -23.94  -20.95    2.99  Cl2
     CO(g)            -48.54   -9.87   38.68  CO
     CO2(g)            -3.84  -11.66   -7.83  CO2
     Dolomite         -13.89  -11.42    2.47  CaMg(CO3)2
     Dolomite-dis     -15.43  -11.42    4.01  CaMg(CO3)2
     Dolomite-ord     -13.88  -11.42    2.46  CaMg(CO3)2
     Epsomite          -8.23  -10.19   -1.96  MgSO4:7H2O
     Gaylussite       -25.74  -14.57   11.16  CaNa2(CO3)2:5H2O
     Glauberite       -18.61  -24.08   -5.47  Na2Ca(SO4)2
     Gypsum            -6.20  -10.73   -4.53  CaSO4:2H2O
     H2(g)            -41.20    1.80   43.00  H2
     H2O(g)            -1.59   -0.00    1.59  H2O
     Halite            -9.61   -8.04    1.56  NaCl
     HCl(g)           -15.88   -9.58    6.30  HCl
     Hexahydrite       -8.47  -10.19   -1.73  MgSO4:6H2O
     Huntite          -32.52  -22.31   10.22  CaMg3(CO3)4
     Hydromagnesite   -46.29  -15.55   30.74  Mg5(CO3)4(OH)2:4H2O
     Hydrophilite     -25.21  -13.47   11.75  CaCl2
     Ice               -0.14   -0.00    0.14  H2O
     K                -69.65    1.33   70.98  K
```

K(g)	-80.25	1.33	81.58	K
K2CO3:1.5H2O	-24.18	-10.80	13.38	K2CO3:1.5H2O
K2O	-83.17	0.87	84.04	K2O
K3H(SO4)2	-27.91	-31.53	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-94.23	-66.52	27.71	K8H4(CO3)6:3H2O
Kainite	-19.03	-19.34	-0.31	KMgClSO4:3H2O
Kalicinite	-11.51	-11.23	0.28	KHCO3
Kieserite	-9.93	-10.19	-0.27	MgSO4:H2O
KMgCl3	-43.32	-22.07	21.25	KMgCl3
KMgCl3:2H2O	-36.04	-22.07	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-19.96	-9.70	10.26	KNaCO3:6H2O
Lansfordite	-10.28	-5.44	4.84	MgCO3:5H2O
Leonite	-21.63	-25.74	-4.11	K2Mg(SO4)2:4H2O
Lime	-26.88	5.69	32.57	CaO
Magnesite	-7.72	-5.44	2.27	MgCO3
Mercallite	-14.54	-15.98	-1.44	KHSO4
Mg	-114.50	8.02	122.52	Mg
Mg(g)	-134.23	8.02	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-13.83	-8.64	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-16.29	-7.08	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-25.66	-12.93	12.73	MgCl2:2H2O
MgCl2:4H2O	-20.23	-12.93	7.30	MgCl2:4H2O
MgCl2:H2O	-29.00	-12.93	16.07	MgCl2:H2O
MgOHCl	-19.25	-3.35	15.89	MgOHCl
MgSO4	-15.02	-10.19	4.83	MgSO4
Mirabilite	-12.19	-13.35	-1.15	Na2SO4:10H2O
Misenite	-100.37	-111.45	-11.08	K8H6(SO4)7
Monohydrocalcite	-8.66	-5.98	2.68	CaCO3:H2O
Na	-64.94	2.43	67.37	Na
Na(g)	-78.43	2.43	80.86	Na
Na2CO3	-19.76	-8.60	11.16	Na2CO3
Na2CO3:7H2O	-18.54	-8.60	9.94	Na2CO3:7H2O
Na2O	-64.35	3.07	67.42	Na2O
Na3H(SO4)2	-27.34	-28.23	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-31.53	-37.43	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-9.99	-10.13	-0.14	NaHCO3
Natron	-18.19	-8.60	9.59	Na2CO3:10H2O
Nesquehonite	-10.73	-5.44	5.29	MgCO3:3H2O
O2(g)	-0.70	-3.59	-2.89	O2
Oxychloride-Mg	-22.97	2.87	25.83	Mg2Cl(OH)3:4H2O
Pentahydrite	-8.81	-10.19	-1.39	MgSO4:5H2O
Periclase	-15.10	6.22	21.33	MgO
Picromerite	-21.30	-25.74	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-25.90	-14.57	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-32.89	-47.20	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-16.86	5.69	22.55	Ca(OH)2
Starkeyite	-9.19	-10.19	-1.00	MgSO4:4H2O
Sylvite	-9.97	-9.14	0.83	KCl
Syngenite	-18.68	-26.28	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-56.47	-39.33	17.14	Mg2CaCl6:12H2O
Thenardite	-12.99	-13.35	-0.36	Na2SO4

```
     Thermonatrite    -19.53   -8.60   10.94  Na2CO3:H2O
     Trona-K          -32.52  -20.93   11.59  K2NaH(CO3)2:2H2O

Initial solution 2.   INEEL Water Quality (CPP-1, 6/6/91)

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

     Elements           Molality       Moles

     C                 3.181e-003  3.181e-003
     Ca                1.348e-003  1.348e-003
     Cl                5.079e-004  5.079e-004
     K                 6.396e-005  6.396e-005
     Mg                5.762e-004  5.762e-004
     Na                3.437e-004  3.437e-004
     O(0)              5.105e-004  5.105e-004  Equilibrium with
O2(g)
     S(6)              2.291e-004  2.291e-004

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

                                        pH  =   8.000
                                        pe  =   8.400
                         Activity of water  =   1.000
                            Ionic strength  =  6.037e-003
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  3.167e-003
                       Total CO2 (mol/kg)   =  3.181e-003
                     Temperature (deg C)    =  25.000
                  Electrical balance (eq)   =  1.228e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =   1.53
                                Iterations  =   5
                                   Total H  = 1.110537e+002
                                   Total O  = 5.553623e+001

--------------------------------Redox couples---------------------
-----------

     Redox couple              pe  Eh (volts)

     O(-2)/O(0)           12.6007      0.7454

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

                                                   Log       Log
Log
     Species            Molality    Activity  Molality  Activity
Gamma
```

```
     OH-                1.047e-006  9.634e-007    -5.980    -6.016
-0.036
     H+                 1.077e-008  1.000e-008    -7.968    -8.000
-0.032
     H2O                5.553e+001  9.999e-001    -0.000    -0.000
0.000
C(-2)             0.000e+000
     C2H4               0.000e+000  0.000e+000  -264.752  -264.752
0.000
C(-3)             0.000e+000
     C2H6               0.000e+000  0.000e+000  -237.066  -237.066
0.000
C(-4)             0.000e+000
     CH4                0.000e+000  0.000e+000  -147.463  -147.463
0.000
C(2)              0.000e+000
     CO                 0.000e+000  0.000e+000   -50.433   -50.433
0.000
C(4)              3.181e-003
     HCO3-              3.020e-003  2.781e-003    -2.520    -2.556
-0.036
     CO2                6.441e-005  6.451e-005    -4.191    -4.190
0.001
     CaHCO3+            3.309e-005  3.047e-005    -4.480    -4.516
-0.036
     CaCO3              2.644e-005  2.644e-005    -4.578    -4.578
0.000
     CO3-2              1.712e-005  1.234e-005    -4.766    -4.909
-0.142
     MgHCO3+            1.403e-005  1.292e-005    -4.853    -4.889
-0.036
     MgCO3              5.221e-006  5.221e-006    -5.282    -5.282
0.000
     NaHCO3             1.253e-006  1.253e-006    -5.902    -5.902
0.000
     NaCO3-             1.477e-008  1.360e-008    -7.831    -7.866
-0.036
Ca                1.348e-003
     Ca+2               1.269e-003  9.247e-004    -2.896    -3.034
-0.138
     CaHCO3+            3.309e-005  3.047e-005    -4.480    -4.516
-0.036
     CaCO3              2.644e-005  2.644e-005    -4.578    -4.578
0.000
     CaSO4              1.890e-005  1.890e-005    -4.724    -4.724
0.000
     CaCl+              9.928e-008  9.143e-008    -7.003    -7.039
-0.036
     CaOH+              1.418e-008  1.306e-008    -7.848    -7.884
-0.036
     CaCl2              5.017e-011  5.017e-011   -10.300   -10.300
0.000
```

```
Cl(-1)          5.079e-004
     Cl-              5.076e-004  4.665e-004    -3.294    -3.331
-0.037
     MgCl+            1.582e-007  1.457e-007    -6.801    -6.837
-0.036
     CaCl+            9.928e-008  9.143e-008    -7.003    -7.039
-0.036
     NaCl             2.583e-008  2.583e-008    -7.588    -7.588
0.000
     KCl              9.198e-010  9.198e-010    -9.036    -9.036
0.000
     CaCl2            5.017e-011  5.017e-011   -10.300   -10.300
0.000
     HCl              1.048e-012  1.048e-012   -11.980   -11.980
0.000
Cl(1)           8.416e-021
     ClO-             6.274e-021  5.777e-021   -20.202   -20.238
-0.036
     HClO             2.143e-021  2.143e-021   -20.669   -20.669
0.000
Cl(3)           9.904e-031
     ClO2-            9.904e-031  9.120e-031   -30.004   -30.040
-0.036
     HClO2            1.348e-035  1.348e-035   -34.870   -34.870
0.000
Cl(5)           1.114e-026
     ClO3-            1.114e-026  1.024e-026   -25.953   -25.990
-0.036
Cl(7)           6.244e-027
     ClO4-            6.244e-027  5.744e-027   -26.205   -26.241
-0.036
H(0)            0.000e+000
     H2               0.000e+000  0.000e+000   -44.302   -44.302
0.001
K               6.396e-005
     K+               6.389e-005  5.872e-005    -4.195    -4.231
-0.037
     KSO4-            7.201e-008  6.631e-008    -7.143    -7.178
-0.036
     KCl              9.198e-010  9.198e-010    -9.036    -9.036
0.000
     KOH              2.036e-011  2.036e-011   -10.691   -10.691
0.000
     KHSO4            5.851e-016  5.851e-016   -15.233   -15.233
0.000
Mg              5.762e-004
     Mg+2             5.418e-004  4.001e-004    -3.266    -3.398
-0.132
     MgSO4            1.495e-005  1.495e-005    -4.825    -4.825
0.000
     MgHCO3+          1.403e-005  1.292e-005    -4.853    -4.889
-0.036
```

```
     MgCO3              5.221e-006  5.221e-006    -5.282    -5.282
0.000
     MgCl+              1.582e-007  1.457e-007    -6.801    -6.837
-0.036
     Mg4(OH)4+4         1.643e-021  4.554e-022   -20.784   -21.342
-0.557
Na               3.437e-004
     Na+                3.421e-004  3.151e-004    -3.466    -3.502
-0.036
     NaHCO3             1.253e-006  1.253e-006    -5.902    -5.902
0.000
     NaSO4-             3.163e-007  2.912e-007    -6.500    -6.536
-0.036
     NaCl               2.583e-008  2.583e-008    -7.588    -7.588
0.000
     NaCO3-             1.477e-008  1.360e-008    -7.831    -7.866
-0.036
     NaOH               5.236e-011  5.236e-011   -10.281   -10.281
0.000
O(0)             5.105e-004
     O2                 2.553e-004  2.556e-004    -3.593    -3.592
0.001
S(6)             2.291e-004
     SO4-2              1.949e-004  1.399e-004    -3.710    -3.854
-0.144
     CaSO4              1.890e-005  1.890e-005    -4.724    -4.724
0.000
     MgSO4              1.495e-005  1.495e-005    -4.825    -4.825
0.000
     NaSO4-             3.163e-007  2.912e-007    -6.500    -6.536
-0.036
     KSO4-              7.201e-008  6.631e-008    -7.143    -7.178
-0.036
     HSO4-              1.535e-010  1.413e-010    -9.814    -9.850
-0.036
     KHSO4              5.851e-016  5.851e-016   -15.233   -15.233
0.000
     H2SO4              1.333e-021  1.333e-021   -20.875   -20.875
0.000

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

     Phase               SI log IAP  log KT

     Anhydrite        -2.54   -6.89   -4.35  CaSO4
     Antarcticite    -13.79   -9.70    4.09  CaCl2:6H2O
     Aphthitalite    -20.02  -23.90   -3.89  NaK3(SO4)2
     Aragonite         0.44    2.41    1.97  CaCO3
     Arcanite        -10.47  -12.32   -1.84  K2SO4
     Artinite         -4.98   14.65   19.63  Mg2CO3(OH)2:3H2O
```

Bassanite	-3.18	-6.89	-3.71	CaSO4:0.5H2O
Bischofite	-14.45	-10.06	4.39	MgCl2:6H2O
Bloedite	-15.63	-18.11	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-3.68	12.60	16.28	Mg(OH)2
Burkeite	-32.76	-23.27	9.49	Na6CO3(SO4)2
C	-71.11	-6.96	64.15	C
C(g)	-188.73	-6.96	181.77	C
Ca	-125.07	14.76	139.83	Ca
Ca(g)	-150.31	14.76	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.02	3.27	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-39.13	29.20	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.59	2.41	1.82	CaCO3
Carnallite	-21.89	-17.62	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-3.35	-6.89	-3.54	CaSO4:0.5H2O
CH4(g)	-144.62	-3.37	141.25	CH4
Chloromagnesite	-31.88	-10.06	21.82	MgCl2
Cl2(g)	-27.45	-24.46	2.99	Cl2
CO(g)	-47.44	-8.76	38.68	CO
CO2(g)	-2.73	-10.56	-7.83	CO2
Dolomite	1.98	4.46	2.47	CaMg(CO3)2
Dolomite-dis	0.44	4.46	4.01	CaMg(CO3)2
Dolomite-ord	1.99	4.46	2.46	CaMg(CO3)2
Epsomite	-5.29	-7.25	-1.96	MgSO4:7H2O
Gaylussite	-10.31	0.85	11.16	CaNa2(CO3)2:5H2O
Glauberite	-12.28	-17.75	-5.47	Na2Ca(SO4)2
Gypsum	-2.36	-6.89	-4.53	CaSO4:2H2O
H2(g)	-41.20	1.80	43.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-8.40	-6.83	1.56	NaCl
HCl(g)	-17.63	-11.33	6.30	HCl
Hexahydrite	-5.53	-7.25	-1.73	MgSO4:6H2O
Huntite	-1.67	8.55	10.22	CaMg3(CO3)4
Hydromagnesite	-9.95	20.79	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.44	-9.70	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-66.31	4.67	70.98	K
K(g)	-76.91	4.67	81.58	K
K2CO3:1.5H2O	-16.40	-3.02	13.38	K2CO3:1.5H2O
K2O	-76.50	7.54	84.04	K2O
K3H(SO4)2	-24.78	-28.40	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-60.89	-33.19	27.71	K8H4(CO3)6:3H2O
Kainite	-14.50	-14.81	-0.31	KMgClSO4:3H2O
Kalicinite	-7.07	-6.79	0.28	KHCO3
Kieserite	-6.99	-7.25	-0.27	MgSO4:H2O
KMgCl3	-38.87	-17.62	21.25	KMgCl3
KMgCl3:2H2O	-31.58	-17.62	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-12.55	-2.29	10.26	KNaCO3:6H2O
Lansfordite	-2.79	2.05	4.84	MgCO3:5H2O
Leonite	-15.46	-19.57	-4.11	K2Mg(SO4)2:4H2O
Lime	-19.60	12.97	32.57	CaO
Magnesite	-0.23	2.05	2.27	MgCO3
Mercallite	-14.65	-16.09	-1.44	KHSO4

```
      Mg                -108.12   14.40  122.52  Mg
      Mg(g)             -127.85   14.40  142.25  Mg
      Mg1.25SO4(OH)0.5:0.5H2O  -9.30   -4.10    5.20
Mg1.25SO4(OH)0.5:0.5H2O
      Mg1.5SO4(OH)      -10.16   -0.95    9.21  Mg1.5SO4(OH)
      MgCl2:2H2O        -22.79  -10.06   12.73  MgCl2:2H2O
      MgCl2:4H2O        -17.36  -10.06    7.30  MgCl2:4H2O
      MgCl2:H2O         -26.13  -10.06   16.07  MgCl2:H2O
      MgOHCl            -14.62    1.27   15.89  MgOHCl
      MgSO4             -12.08   -7.25    4.83  MgSO4
      Mirabilite         -9.70  -10.86   -1.15  Na2SO4:10H2O
      Misenite          -97.75 -108.83  -11.08  K8H6(SO4)7
      Monohydrocalcite   -0.27    2.41    2.68  CaCO3:H2O
      Na                -61.97    5.40   67.37  Na
      Na(g)             -75.46    5.40   80.86  Na
      Na2CO3            -12.72   -1.56   11.16  Na2CO3
      Na2CO3:7H2O       -11.50   -1.56    9.94  Na2CO3:7H2O
      Na2O              -58.42    9.00   67.42  Na2O
      Na3H(SO4)2        -25.32  -26.21   -0.89  Na3H(SO4)2
      Na4Ca(SO4)3:2H2O -22.71  -28.60   -5.89  Na4Ca(SO4)3:2H2O
      Nahcolite          -5.92   -6.06   -0.14  NaHCO3
      Natron            -11.15   -1.56    9.59  Na2CO3:10H2O
      Nesquehonite       -3.24    2.05    5.29  MgCO3:3H2O
      O2(g)              -0.70   -3.59   -2.89  O2
      Oxychloride-Mg    -11.96   13.87   25.83  Mg2Cl(OH)3:4H2O
      Pentahydrite       -5.87   -7.25   -1.39  MgSO4:5H2O
      Periclase          -8.72   12.60   21.33  MgO
      Picromerite       -15.13  -19.57   -4.44  K2Mg(SO4)2:6H2O
      Pirssonite        -10.47    0.85   11.32  Na2Ca(CO3)2:2H2O
      Polyhalite        -19.03  -33.35  -14.31  K2MgCa2(SO4)4:2H2O
      Portlandite        -9.58   12.97   22.55  Ca(OH)2
      Starkeyite         -6.25   -7.25   -1.00  MgSO4:4H2O
      Sylvite            -8.39   -7.56    0.83  KCl
      Syngenite         -11.60  -19.20   -7.60  K2Ca(SO4)2:H2O
      Tachyhydrite      -46.96  -29.82   17.14  Mg2CaCl6:12H2O
      Thenardite        -10.50  -10.86   -0.36  Na2SO4
      Thermonatrite     -12.50   -1.56   10.94  Na2CO3:H2O
      Trona-K           -20.66   -9.08   11.59  K2NaH(CO3)2:2H2O

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

Reaction step 1.

Using mix 1.     Mixing Solutions 1 and 2

Mixture 1. Mixing Solutions 1 and 2

       7.400e-001 Solution 1      Average Rainfall Composition
       2.600e-001 Solution 2      INEEL Water Quality (CPP-1, 6/6/91)
```

```
-----------------------------Solution composition-------------------
-----------

     Elements            Molality       Moles

     C                 8.315e-004  8.315e-004
     Ca                3.528e-004  3.528e-004
     Cl                2.114e-004  2.114e-004
     K                 2.174e-005  2.174e-005
     Mg                1.580e-004  1.580e-004
     Na                1.537e-004  1.537e-004
     S                 6.435e-005  6.435e-005

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

                                        pH  =   8.009      Charge
balance
                                        pe  =  12.591      Adjusted
to redox equilibrium
                        Activity of water  =   1.000
                           Ionic strength  =  1.727e-003
                       Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  8.221e-004
                       Total CO2 (mol/kg)  =  8.315e-004
                     Temperature (deg C)   =  25.000
                  Electrical balance (eq)  =  3.502e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   1.51
                               Iterations  =  24
                                  Total H  = 1.110515e+002
                                  Total O  = 5.552857e+001

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

                                                   Log       Log
Log
     Species             Molality    Activity  Molality  Activity
Gamma

     OH-               1.031e-006  9.845e-007    -5.987    -6.007
-0.020
     H+                1.022e-008  9.786e-009    -7.991    -8.009
-0.019
     H2O               5.553e+001  1.000e+000    -0.000    -0.000
0.000
C(-2)            0.000e+000
     C2H4              0.000e+000  0.000e+000  -265.890  -265.890
0.000
C(-3)            0.000e+000
     C2H6              0.000e+000  0.000e+000  -238.204  -238.204
0.000
```

```
C(-4)            0.000e+000
     CH4                 0.000e+000  0.000e+000  -148.032  -148.032
0.000
C(2)             0.000e+000
     CO                  0.000e+000  0.000e+000   -51.002   -51.002
0.000
C(4)             8.315e-004
     HCO3-               8.030e-004  7.667e-004    -3.095    -3.115
-0.020
     CO2                 1.740e-005  1.740e-005    -4.760    -4.759
0.000
     CO3-2               4.179e-006  3.476e-006    -5.379    -5.459
-0.080
     CaHCO3+             2.745e-006  2.621e-006    -5.561    -5.582
-0.020
     CaCO3               2.324e-006  2.324e-006    -5.634    -5.634
0.000
     MgHCO3+             1.209e-006  1.154e-006    -5.918    -5.938
-0.020
     MgCO3               4.765e-007  4.765e-007    -6.322    -6.322
0.000
     NaHCO3              1.608e-007  1.608e-007    -6.794    -6.794
0.000
     NaCO3-              1.867e-009  1.783e-009    -8.729    -8.749
-0.020
Ca               3.528e-004
     Ca+2                3.456e-004  2.885e-004    -3.461    -3.540
-0.078
     CaHCO3+             2.745e-006  2.621e-006    -5.561    -5.582
-0.020
     CaCO3               2.324e-006  2.324e-006    -5.634    -5.634
0.000
     CaSO4               2.116e-006  2.116e-006    -5.675    -5.675
0.000
     CaCl+               1.291e-008  1.233e-008    -7.889    -7.909
-0.020
     CaOH+               4.361e-009  4.164e-009    -8.360    -8.381
-0.020
     CaCl2               2.924e-012  2.924e-012   -11.534   -11.534
0.000
Cl(-1)           2.114e-004
     Cl-                 2.113e-004  2.017e-004    -3.675    -3.695
-0.020
     MgCl+               2.137e-008  2.040e-008    -7.670    -7.690
-0.020
     CaCl+               1.291e-008  1.233e-008    -7.889    -7.909
-0.020
     NaCl                5.196e-009  5.196e-009    -8.284    -8.284
0.000
     KCl                 1.404e-010  1.404e-010    -9.853    -9.853
0.000
```

```
     CaCl2              2.924e-012  2.924e-012   -11.534   -11.534
0.000
     HCl                4.432e-013  4.432e-013   -12.353   -12.353
0.000
Cl(1)             3.522e-021
     ClO-               2.616e-021  2.497e-021   -20.582   -20.603
-0.020
     HClO               9.063e-022  9.063e-022   -21.043   -21.043
0.000
Cl(3)             4.129e-031
     ClO2-              4.129e-031  3.942e-031   -30.384   -30.404
-0.020
     HClO2              5.704e-036  5.704e-036   -35.244   -35.244
0.000
Cl(5)             4.639e-027
     ClO3-              4.639e-027  4.428e-027   -26.334   -26.354
-0.020
Cl(7)             2.601e-027
     ClO4-              2.601e-027  2.483e-027   -26.585   -26.605
-0.020
H(0)              0.000e+000
     H2                 0.000e+000  0.000e+000   -44.302   -44.302
0.000
K                 2.174e-005
     K+                 2.173e-005  2.074e-005    -4.663    -4.683
-0.020
     KSO4-              8.802e-009  8.404e-009    -8.055    -8.076
-0.020
     KCl                1.404e-010  1.404e-010    -9.853    -9.853
0.000
     KOH                7.347e-012  7.347e-012   -11.134   -11.134
0.000
     KHSO4              7.256e-017  7.256e-017   -16.139   -16.139
0.000
Mg                1.580e-004
     Mg+2               1.546e-004  1.296e-004    -3.811    -3.887
-0.077
     MgSO4              1.738e-006  1.738e-006    -5.760    -5.760
0.000
     MgHCO3+            1.209e-006  1.154e-006    -5.918    -5.938
-0.020
     MgCO3              4.765e-007  4.765e-007    -6.322    -6.322
0.000
     MgCl+              2.137e-008  2.040e-008    -7.670    -7.690
-0.020
     Mg4(OH)4+4         1.133e-023  5.470e-024   -22.946   -23.262
-0.316
Na                1.537e-004
     Na+                1.535e-004  1.466e-004    -3.814    -3.834
-0.020
     NaHCO3             1.608e-007  1.608e-007    -6.794    -6.794
0.000
```

```
     NaSO4-            5.093e-008  4.863e-008    -7.293    -7.313
-0.020
     NaCl              5.196e-009  5.196e-009    -8.284    -8.284
0.000
     NaCO3-            1.867e-009  1.783e-009    -8.729    -8.749
-0.020
     NaOH              2.490e-011  2.490e-011   -10.604   -10.604
0.000
O(0)             5.111e-004
     O2                2.555e-004  2.557e-004    -3.593    -3.592
0.000
     S3O6-2            0.000e+000  0.000e+000  -183.662  -183.742
-0.081
     S2-2              0.000e+000  0.000e+000  -255.271  -255.352
-0.081
     S4O6-2            0.000e+000  0.000e+000  -277.309  -277.389
-0.081
     S3-2              0.000e+000  0.000e+000  -362.341  -362.421
-0.081
     S5O6-2            0.000e+000  0.000e+000  -399.835  -399.916
-0.081
     S4-2              0.000e+000  0.000e+000  -469.638  -469.718
-0.081
     S5-2              0.000e+000  0.000e+000  -577.151  -577.232
-0.081
S(-2)            0.000e+000
     HS-               0.000e+000  0.000e+000  -143.386  -143.406
-0.020
     H2S               0.000e+000  0.000e+000  -144.406  -144.406
0.000
     S-2               0.000e+000  0.000e+000  -148.244  -148.323
-0.080
     S2-2              0.000e+000  0.000e+000  -255.271  -255.352
-0.081
     S3-2              0.000e+000  0.000e+000  -362.341  -362.421
-0.081
     S4-2              0.000e+000  0.000e+000  -469.638  -469.718
-0.081
     S5-2              0.000e+000  0.000e+000  -577.151  -577.232
-0.081
S(2)             0.000e+000
     S2O3-2            0.000e+000  0.000e+000  -150.826  -150.906
-0.081
     HS2O3-            0.000e+000  0.000e+000  -157.882  -157.902
-0.020
S(3)             0.000e+000
     S2O4-2            0.000e+000  0.000e+000  -140.048  -140.127
-0.080
S(4)             0.000e+000
     SO3-2             0.000e+000  0.000e+000   -49.041   -49.121
-0.080
```

```
     HSO3-              0.000e+000  0.000e+000   -49.879   -49.899
-0.020
     H2SO3              0.000e+000  0.000e+000   -55.926   -55.926
0.000
     SO2                0.000e+000  0.000e+000   -56.027   -56.027
0.000
     S2O5-2             0.000e+000  0.000e+000  -104.547  -104.628
-0.081
     S3O6-2             0.000e+000  0.000e+000  -183.662  -183.742
-0.081
     S4O6-2             0.000e+000  0.000e+000  -277.309  -277.389
-0.081
     S5O6-2             0.000e+000  0.000e+000  -399.835  -399.916
-0.081
S(5)            0.000e+000
     S2O6-2             0.000e+000  0.000e+000   -74.109   -74.190
-0.081
S(6)            6.435e-005
     SO4-2              6.044e-005  5.021e-005    -4.219    -4.299
-0.081
     CaSO4              2.116e-006  2.116e-006    -5.675    -5.675
0.000
     MgSO4              1.738e-006  1.738e-006    -5.760    -5.760
0.000
     NaSO4-             5.093e-008  4.863e-008    -7.293    -7.313
-0.020
     KSO4-              8.802e-009  8.404e-009    -8.055    -8.076
-0.020
     HSO4-              5.198e-011  4.963e-011   -10.284   -10.304
-0.020
     KHSO4              7.256e-017  7.256e-017   -16.139   -16.139
0.000
     H2SO4              4.583e-022  4.583e-022   -21.339   -21.339
0.000
S(7)            0.000e+000
     S2O8-2             0.000e+000  0.000e+000   -48.788   -48.868
-0.081
S(8)            4.515e-032
     HSO5-              4.515e-032  4.311e-032   -31.345   -31.365
-0.020

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

     Phase               SI log IAP  log KT

     Anhydrite        -3.49   -7.84   -4.35  CaSO4
     Antarcticite    -15.02  -10.93    4.09  CaCl2:6H2O
     Aphthitalite    -22.59  -26.48   -3.89  NaK3(SO4)2
     Aragonite        -0.62    1.35    1.97  CaCO3
     Arcanite        -11.82  -13.67   -1.84  K2SO4
     Artinite         -6.49   13.14   19.63  Mg2CO3(OH)2:3H2O
```

Bassanite	-4.13	-7.84	-3.71	CaSO4:0.5H2O
Bischofite	-15.67	-11.28	4.39	MgCl2:6H2O
Bloedite	-17.68	-20.15	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-4.15	12.13	16.28	Mg(OH)2
Burkeite	-36.19	-26.71	9.49	Na6CO3(SO4)2
C	-71.68	-93.53	-21.85	C
C(g)	-189.30	-93.53	95.77	C
Ca	-125.56	-28.72	96.83	Ca
Ca(g)	-150.80	-28.72	122.07	Ca
Ca2Cl2(OH)2:H2O	-24.74	1.55	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-41.82	26.51	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-0.47	1.35	1.82	CaCO3
Carnallite	-23.93	-19.66	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-4.30	-7.84	-3.54	CaSO4:0.5H2O
CH4(g)	-145.19	-175.93	-30.74	CH4
Chloromagnesite	-33.09	-11.28	21.82	MgCl2
Cl2(g)	-28.20	17.79	45.99	Cl2
CO(g)	-48.01	-52.33	-4.32	CO
CO2(g)	-3.30	-11.12	-7.83	CO2
Dolomite	-0.11	2.36	2.47	CaMg(CO3)2
Dolomite-dis	-1.65	2.36	4.01	CaMg(CO3)2
Dolomite-ord	-0.10	2.36	2.46	CaMg(CO3)2
Epsomite	-6.22	-8.19	-1.96	MgSO4:7H2O
Gaylussite	-12.58	-1.42	11.16	CaNa2(CO3)2:5H2O
Glauberite	-14.34	-19.81	-5.47	Na2Ca(SO4)2
Gypsum	-3.31	-7.84	-4.53	CaSO4:2H2O
H2(g)	-41.20	-41.20	-0.00	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-143.42	-185.12	-41.70	H2S
Halite	-9.09	-7.53	1.56	NaCl
HCl(g)	-18.01	-11.70	6.30	HCl
Hexahydrite	-6.46	-8.19	-1.73	MgSO4:6H2O
Huntite	-5.84	4.37	10.22	CaMg3(CO3)4
Hydromagnesite	-14.58	16.16	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-22.68	-10.93	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
K	-66.75	-17.27	49.48	K
K(g)	-77.35	-17.27	60.08	K
K2CO3:1.5H2O	-17.85	-4.47	13.38	K2CO3:1.5H2O
K2O	-77.38	6.65	84.04	K2O
K3H(SO4)2	-27.03	-30.66	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-67.85	-40.14	27.71	K8H4(CO3)6:3H2O
Kainite	-16.25	-16.57	-0.31	KMgClSO4:3H2O
Kalicinite	-8.08	-7.80	0.28	KHCO3
Kieserite	-7.92	-8.19	-0.27	MgSO4:H2O
KMgCl3	-40.90	-19.66	21.25	KMgCl3
KMgCl3:2H2O	-33.62	-19.66	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-13.88	-3.62	10.26	KNaCO3:6H2O
Lansfordite	-3.83	1.01	4.84	MgCO3:5H2O
Leonite	-17.74	-21.85	-4.11	K2Mg(SO4)2:4H2O
Lime	-20.09	12.48	32.57	CaO
Magnesite	-1.27	1.01	2.27	MgCO3

```
     Mercallite        -15.55  -16.99   -1.44  KHSO4
     Mg               -108.59  -29.07   79.52  Mg
     Mg(g)            -128.32  -29.07   99.25  Mg
     Mg1.25SO4(OH)0.5:0.5H2O -10.35   -5.15    5.20
Mg1.25SO4(OH)0.5:0.5H2O
     Mg1.5SO4(OH)      -11.33   -2.12    9.21  Mg1.5SO4(OH)
     MgCl2:2H2O        -24.01  -11.28   12.73  MgCl2:2H2O
     MgCl2:4H2O        -18.58  -11.28    7.30  MgCl2:4H2O
     MgCl2:H2O         -27.35  -11.28   16.07  MgCl2:H2O
     MgOHCl            -15.46    0.43   15.89  MgOHCl
     MgSO4             -13.01   -8.19    4.83  MgSO4
     Mirabilite        -10.81  -11.97   -1.15  Na2SO4:10H2O
     Misenite         -104.54 -115.62  -11.08  K8H6(SO4)7
     Monohydrocalcite  -1.32    1.35    2.68  CaCO3:H2O
     Na                -62.30  -16.43   45.87  Na
     Na(g)             -75.79  -16.43   59.36  Na
     Na2CO3            -13.94   -2.77   11.16  Na2CO3
     Na2CO3:7H2O       -12.71   -2.77    9.94  Na2CO3:7H2O
     Na2O              -59.07    8.35   67.42  Na2O
     Na3H(SO4)2        -27.22  -28.11   -0.89  Na3H(SO4)2
     Na4Ca(SO4)3:2H2O -25.88  -31.77   -5.89  Na4Ca(SO4)3:2H2O
     Nahcolite          -6.81   -6.95   -0.14  NaHCO3
     Natron            -12.36   -2.77    9.59  Na2CO3:10H2O
     Nesquehonite       -4.28    1.01    5.29  MgCO3:3H2O
     O2(g)              -0.70   82.40   83.10  O2
     Oxychloride-Mg    -13.27   12.56   25.83  Mg2Cl(OH)3:4H2O
     Pentahydrite       -6.80   -8.19   -1.39  MgSO4:5H2O
     Periclase          -9.19   12.13   21.33  MgO
     Picromerite       -17.41  -21.85   -4.44  K2Mg(SO4)2:6H2O
     Pirssonite        -12.74   -1.42   11.32  Na2Ca(CO3)2:2H2O
     Polyhalite        -23.22  -37.53  -14.31  K2MgCa2(SO4)4:2H2O
     Portlandite       -10.07   12.48   22.55  Ca(OH)2
     S                -108.10 -143.92  -35.82  S
     S2(g)            -230.10 -287.84  -57.75  S2
     SO2(g)            -56.20  -61.52   -5.32  SO2
     Starkeyite         -7.19   -8.19   -1.00  MgSO4:4H2O
     Sylvite            -9.21   -8.38    0.83  KCl
     Syngenite         -13.90  -21.50   -7.60  K2Ca(SO4)2:H2O
     Tachyhydrite      -50.63  -33.49   17.14  Mg2CaCl6:12H2O
     Thenardite        -11.61  -11.97   -0.36  Na2SO4
     Thermonatrite     -13.71   -2.77   10.94  Na2CO3:H2O
     Trona-K           -23.01  -11.42   11.59  K2NaH(CO3)2:2H2O

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

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

     USE SOLUTION  3
```

```
REACTION
NaCN  2.16e-04
NaI   9.49e-07
1.0
EQUILIBRIUM_PHASES 1
Calcite     0.0  6.1
Illite      0.0   4.1
Kaolinite  0.0  0.0
Quartz      0.0  106.5
Gypsum      0.0   0.0013
Albite      0.0  14.4
K-Feldspar  0.0  7.8
Fluorapatite  0.0  0.017
Dolomite  0.0   Enstatite  21.7
Yb2O3  0.0  0.0094
Fe(OH)3  0.0  2.89
Pyrite  0.0  0.17
Zincite  0.0  Sphalerite  0.05
Birnessite  0.0  0.008
Barite  0.0  0.022
Borax  0.0  0.07
PuO2   0.0  8.76e-09
CaUO4  0.0  0.000417
Ca2V2O7  0.0  0.0035
Tb2O3    0.0  0.03
TcO2:2H2O(am)   0.0  5.72e-08
Ca3(AsO4)2  0.0  0.0006
Niter  0.0  0.001
Halite    0.0  0.0009
CaSeO4    0.0  1.8e-04
O2(g)   -0.7   1.0
CO2(g)    -3.5   1.0
END
-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 3.     Solution after simulation 1.
Using pure phase assemblage 1.
Using reaction 1.

Reaction 1.     Irreversible reaction defined in simulation 2.

      1.000e+000 moles of the following reaction have been added:

                        Relative
     Reactant              moles

     NaCN                   0.00
     NaI                    0.00
```

Element	Relative moles
C	0.00
I	0.00
N	0.00
Na	0.00

----------Phase assemblage----------

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Albite	0.00	2.66	2.66	1.440e+001	1.418e+001	-2.237e-001
Barite	0.00	-10.01	-10.01	2.200e-002	2.200e-002	-1.923e-008
Birnessite	0.00	269.79	269.79	8.000e-003	8.000e-003	-7.118e-014
Borax	-0.00	12.04	12.04	7.000e-002	1.221e-002	-5.779e-002
Ca2V2O7	-0.47	16.71	17.18	3.500e-003	-	3.500e-003
Ca3(AsO4)2	-53.49	-35.69	17.80	6.000e-004	-	6.000e-004
Calcite	-0.00	1.82	1.82	6.100e+000	5.975e+000	-1.252e-001
CaSeO4	-4.28	-7.37	-3.09	1.800e-004	-	1.800e-004
CaUO4	0.00	15.94	15.94	4.170e-004	4.136e-004	-3.406e-006
CO2(g)	-3.50	-11.33	-7.83	1.000e+000	1.063e+000	6.339e-002
Dolomite	-0.00	2.47	2.47			
MgSiO3	is reactant			2.170e+001	2.272e+001	1.024e+000
Fe(OH)3	0.00	18.66	18.66	2.890e+000	3.060e+000	1.700e-001
Fluorapatite	-0.00	-25.16	-25.16	1.700e-002	1.580e-002	-1.200e-003
Gypsum	0.00	-4.53	-4.53	1.300e-003	1.315e-001	1.302e-001
Halite	-5.38	-3.81	1.56	9.000e-004	-	9.000e-004
Illite	-0.40	8.48	8.88	4.100e+000	-	4.100e+000
K-Feldspar	-0.00	-0.38	-0.38	7.800e+000	1.026e+001	2.461e+000

```
     Kaolinite          0.00    6.72    6.72 0.000e+000 3.597e+000
3.597e+000
     Niter             -6.58   -6.81   -0.22 1.000e-003           -
1.000e-003
     O2(g)             -0.70   82.40   83.10 1.000e+000 3.618e-001-
6.382e-001
     PuO2               0.00  -25.93  -25.93 8.760e-009 8.760e-009-
2.901e-013
     Pyrite          -242.00 -325.69  -83.69 1.700e-001           -
1.700e-001
     Quartz             0.00   -4.03   -4.03 1.065e+002 1.059e+002-
5.783e-001
     Tb2O3             -7.09   40.01   47.10 3.000e-002           -
3.000e-002
     TcO2:2H2O(am)    -40.01  -77.23  -37.22 5.720e-008           -
5.720e-008
     Yb2O3             -9.39   38.41   47.80 9.400e-003           -
9.400e-003
     Zincite            0.00   11.20   11.20
          ZnS              is reactant    5.000e-002 4.988e-002-
1.208e-004

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

     Elements           Molality       Moles

     Al               5.292e-008  4.972e-008
     As               1.277e-003  1.200e-003
     B                2.460e-001  2.311e-001
     Ba               2.047e-008  1.923e-008
     C                6.685e-002  6.281e-002
     Ca               1.094e-002  1.028e-002
     Cl               1.183e-003  1.111e-003
     F                1.277e-003  1.200e-003
     Fe               4.660e-007  4.378e-007
     I                1.010e-006  9.490e-007
     K                3.562e-004  3.346e-004
     Mg               9.261e-004  8.701e-004
     Mn               6.061e-013  5.694e-013
     N                1.294e-003  1.216e-003
     Na               3.625e-001  3.406e-001
     P                3.832e-003  3.600e-003
     Pu               3.088e-013  2.901e-013
     S                2.235e-001  2.100e-001
     Se               1.916e-004  1.800e-004
     Si               1.066e-004  1.002e-004
     Tb               6.386e-002  6.000e-002
     Tc               6.088e-008  5.720e-008
     U                3.625e-006  3.406e-006
     V                7.451e-003  7.000e-003
     Yb               2.001e-002  1.880e-002
```

```
     Zn                1.286e-004  1.208e-004

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

                                        pH  =   8.032      Charge
balance
                                        pe  =  12.571      Adjusted
to redox equilibrium
                        Activity of water  =   0.986
                           Ionic strength  =  5.454e-001
                       Mass of water (kg)  =  9.395e-001
                 Total alkalinity (eq/kg)  =  1.935e-001
                       Total CO2 (mol/kg)  =  6.685e-002
                     Temperature (deg C)   =  25.000
                  Electrical balance (eq)  =  3.502e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                                Iterations  =  29
                                   Total H  = 1.049903e+002
                                   Total O  = 5.392986e+001

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

                                                   Log       Log
Log
     Species            Molality    Activity  Molality  Activity
Gamma

     OH-              1.555e-006  1.023e-006    -5.808    -5.990
-0.182
     H+               1.158e-008  9.281e-009    -7.936    -8.032
-0.096
     H2O              5.553e+001  9.856e-001    -0.006    -0.006
0.000
Al               5.292e-008
     AlO2-            5.062e-008  3.429e-008    -7.296    -7.465
-0.169
     NaAlO2           1.363e-009  1.363e-009    -8.866    -8.866
0.000
     HAlO2            9.289e-010  9.289e-010    -9.032    -9.032
0.000
     Al(OH)2+         8.747e-012  5.924e-012   -11.058   -11.227
-0.169
     AlOH+2           1.203e-013  2.403e-014   -12.920   -13.619
-0.700
     Al(SO4)2-        1.404e-015  9.508e-016   -14.853   -15.022
-0.169
     AlSO4+           7.428e-016  5.031e-016   -15.129   -15.298
-0.169
     Al+3             2.239e-016  2.019e-017   -15.650   -16.695
-1.045
```

```
     AlHPO4+          1.197e-016  8.109e-017   -15.922   -16.091
-0.169
     Al2(OH)2+4       3.447e-023  9.386e-026   -22.462   -25.028
-2.565
     AlF+2            4.639e-024  9.267e-025   -23.334   -24.033
-0.700
     AlH2PO4+2        1.889e-028  3.772e-029   -27.724   -28.423
-0.700
     Al3(OH)4+5       9.130e-029  1.380e-032   -28.040   -31.860
-3.821
     AlF2+            2.499e-033  1.693e-033   -32.602   -32.771
-0.169
     AlF3             0.000e+000  0.000e+000   -43.010   -43.010
0.000
     Al13O4(OH)24+7   0.000e+000  0.000e+000   -51.392   -58.901
-7.510
     AlF4-            0.000e+000  0.000e+000   -54.779   -54.948
-0.169
As(-3)          0.000e+000
     AsH3             0.000e+000  0.000e+000  -185.600  -185.600
0.000
As(3)           0.000e+000
     HAsO2            0.000e+000  0.000e+000   -57.042   -57.042
0.000
     As(OH)3          0.000e+000  0.000e+000   -57.106   -57.106
0.000
     H2AsO3-          0.000e+000  0.000e+000   -58.118   -58.288
-0.169
     AsO2-            0.000e+000  0.000e+000   -58.132   -58.301
-0.169
     AsO2OH-2         0.000e+000  0.000e+000   -60.521   -61.265
-0.744
     HAsS2            0.000e+000  0.000e+000  -333.373  -333.373
0.000
As(5)           1.277e-003
     AsO3F-2          1.275e-003  2.299e-004    -2.895    -3.639
-0.744
     HAsO3F-          2.339e-006  1.584e-006    -5.631    -5.800
-0.169
     HAsO4-2          2.785e-028  5.022e-029   -27.555   -28.299
-0.744
     H2AsO4-          4.146e-030  2.808e-030   -29.382   -29.552
-0.169
     AsO4-3           6.989e-031  1.388e-032   -30.156   -31.858
-1.702
     H3AsO4           4.591e-036  4.591e-036   -35.338   -35.338
0.000
B(-5)           0.000e+000
     BH4-             0.000e+000  0.000e+000  -222.362  -222.531
-0.169
B(3)            2.460e-001
```

```
     B(OH)3            2.201e-001  2.201e-001    -0.657    -0.657
0.000
     BO2-              1.904e-002  1.290e-002    -1.720    -1.889
-0.169
     NaB(OH)4          5.169e-003  5.169e-003    -2.287    -2.287
0.000
     CaB(OH)4+         1.624e-003  1.100e-003    -2.789    -2.959
-0.169
     MgB(OH)4+         1.288e-004  8.725e-005    -3.890    -4.059
-0.169
     BaB(OH)4+         2.178e-009  1.475e-009    -8.662    -8.831
-0.169
     B2O(OH)5-         1.591e-012  1.077e-012   -11.798   -11.968
-0.169
     BF2(OH)2-         2.669e-031  1.808e-031   -30.574   -30.743
-0.169
     BF3OH-            0.000e+000  0.000e+000   -46.308   -46.477
-0.169
     BF4-              0.000e+000  0.000e+000   -63.851   -64.020
-0.169
Ba               2.047e-008
     Ba+2              1.825e-008  3.993e-009    -7.739    -8.399
-0.660
     BaB(OH)4+         2.178e-009  1.475e-009    -8.662    -8.831
-0.169
     BaNO3+            3.832e-011  2.596e-011   -10.417   -10.586
-0.169
     BaCO3             4.646e-012  4.646e-012   -11.333   -11.333
0.000
     BaCl+             1.454e-012  9.849e-013   -11.837   -12.007
-0.169
     BaOH+             2.122e-014  1.437e-014   -13.673   -13.843
-0.169
     BaF+              1.864e-023  1.262e-023   -22.730   -22.899
-0.169
C(-2)            0.000e+000
     C2H4              0.000e+000  0.000e+000  -266.310  -266.310
0.000
C(-3)            0.000e+000
     C2H6              0.000e+000  0.000e+000  -238.631  -238.631
0.000
C(-4)            0.000e+000
     CH4               0.000e+000  0.000e+000  -148.248  -148.248
0.000
C(2)             0.000e+000
     CO                0.000e+000  0.000e+000   -51.206   -51.206
0.000
C(4)             6.685e-002
     TbCO3+            2.687e-002  1.820e-002    -1.571    -1.740
-0.169
     YbCO3+            9.875e-003  6.688e-003    -2.005    -2.175
-0.169
```

Tb(CO3)2-	9.715e-003	6.580e-003	-2.013	-2.182	-0.169
Yb(CO3)2-	4.866e-003	3.296e-003	-2.313	-2.482	-0.169
HCO3-	7.357e-004	4.982e-004	-3.133	-3.303	-0.169
NaHCO3	1.485e-004	1.485e-004	-3.828	-3.828	0.000
CO3-2	1.192e-005	2.382e-006	-4.924	-5.623	-0.700
TbHCO3+2	1.097e-005	2.191e-006	-4.960	-5.659	-0.700
CaHCO3+	1.085e-005	7.345e-006	-4.965	-5.134	-0.169
CO2	9.594e-006	1.088e-005	-5.018	-4.963	0.055
CaCO3	6.867e-006	6.867e-006	-5.163	-5.163	0.000
UO2(CO3)3-4	3.426e-006	3.103e-009	-5.465	-8.508	-3.043
NaCO3-	2.564e-006	1.736e-006	-5.591	-5.760	-0.169
YbHCO3+2	2.413e-006	4.819e-007	-5.617	-6.317	-0.700
MgHCO3+	7.088e-007	4.800e-007	-6.149	-6.319	-0.169
ZnCO3	2.765e-007	2.765e-007	-6.558	-6.558	0.000
ZnHCO3+	2.621e-007	1.775e-007	-6.582	-6.751	-0.169
MgCO3	2.090e-007	2.090e-007	-6.680	-6.680	0.000
UO2(CO3)2-2	1.606e-007	2.895e-008	-6.794	-7.538	-0.744
(UO2)2CO3(OH)3-	1.589e-009	1.076e-009	-8.799	-8.968	-0.169
UO2CO3	6.320e-010	6.320e-010	-9.199	-9.199	0.000
BaCO3	4.646e-012	4.646e-012	-11.333	-11.333	0.000
(UO2)3(CO3)6-6	2.591e-013	3.456e-020	-12.587	-19.461	-6.875
PuO2(CO3)2-2	2.396e-013	4.320e-014	-12.621	-13.365	-0.744
FeCO3+	7.391e-015	5.006e-015	-14.131	-14.301	-0.169
MnCO3	4.895e-015	4.895e-015	-14.310	-14.310	0.000
MnHCO3+	3.288e-016	2.227e-016	-15.483	-15.652	-0.169
FeHCO3+	3.931e-019	2.663e-019	-18.405	-18.575	-0.169

```
     FeCO3              1.377e-019  1.377e-019   -18.861   -18.861
0.000
     (UO2)3(OH)5CO2+  3.324e-021  2.251e-021   -20.478   -20.648
-0.169
     (UO2)3O(OH)2(HCO3)+  2.719e-021  1.842e-021   -20.566   -
20.735    -0.169
     UO2(CO3)3-5        9.236e-030  1.578e-034   -29.035   -33.802
-4.767
     U(CO3)4-4          0.000e+000  0.000e+000   -45.777   -48.820
-3.043
     (UO2)11(CO3)6(OH)12-2  0.000e+000  0.000e+000   -46.342   -
47.086    -0.744
     U(CO3)5-6          0.000e+000  0.000e+000   -48.651   -55.526
-6.875
     SCN-               0.000e+000  0.000e+000  -214.854  -215.036
-0.182
     UO2SCN+            0.000e+000  0.000e+000  -226.733  -226.902
-0.169
     USCN+3             0.000e+000  0.000e+000  -272.031  -273.544
-1.513
     Zn(SCN)2           0.000e+000  0.000e+000  -434.051  -434.051
0.000
     UO2(SCN)2          0.000e+000  0.000e+000  -442.106  -442.106
0.000
     U(SCN)2+2          0.000e+000  0.000e+000  -486.579  -487.279
-0.700
     UO2(SCN)3-         0.000e+000  0.000e+000  -656.113  -656.282
-0.169
     Zn(SCN)4-2         0.000e+000  0.000e+000  -863.011  -863.755
-0.744
Ca                1.094e-002
     Ca+2               4.868e-003  1.244e-003    -2.313    -2.905
-0.593
     CaSO4              4.424e-003  4.424e-003    -2.354    -2.354
0.000
     CaB(OH)4+          1.624e-003  1.100e-003    -2.789    -2.959
-0.169
     CaHCO3+            1.085e-005  7.345e-006    -4.965    -5.134
-0.169
     CaNO3+             7.534e-006  5.102e-006    -5.123    -5.292
-0.169
     CaCO3              6.867e-006  6.867e-006    -5.163    -5.163
0.000
     CaCl+              2.862e-007  1.939e-007    -6.543    -6.712
-0.169
     CaHPO4             1.093e-007  1.093e-007    -6.961    -6.961
0.000
     CaPO4-             4.349e-008  2.946e-008    -7.362    -7.531
-0.169
     CaOH+              2.755e-008  1.866e-008    -7.560    -7.729
-0.169
```

```
     CaCl2              1.676e-010  1.676e-010    -9.776    -9.776
0.000
     CaP2O7-2           2.025e-013  3.650e-014   -12.694   -13.438
-0.744
     CaH2PO4+           6.846e-017  4.637e-017   -16.165   -16.334
-0.169
     CaF+               4.284e-017  2.902e-017   -16.368   -16.537
-0.169
Cl(-1)            1.183e-003
     Cl-                1.155e-003  7.352e-004    -2.937    -3.134
-0.196
     NaCl               2.692e-005  2.692e-005    -4.570    -4.570
0.000
     TbCl+2             5.515e-007  1.102e-007    -6.258    -6.958
-0.700
     CaCl+              2.862e-007  1.939e-007    -6.543    -6.712
-0.169
     YbCl+2             7.390e-008  1.476e-008    -7.131    -7.831
-0.700
     MgCl+              7.030e-008  4.761e-008    -7.153    -7.322
-0.169
     Zn(OH)Cl           3.100e-008  3.100e-008    -7.509    -7.509
0.000
     ZnCl+              2.521e-008  1.707e-008    -7.598    -7.768
-0.169
     KCl                4.725e-009  4.725e-009    -8.326    -8.326
0.000
     CaCl2              1.676e-010  1.676e-010    -9.776    -9.776
0.000
     TbCl2+             6.547e-011  4.434e-011   -10.184   -10.353
-0.169
     ZnCl2              1.466e-011  1.466e-011   -10.834   -10.834
0.000
     YbCl2+             6.349e-012  4.300e-012   -11.197   -11.367
-0.169
     HCl                1.533e-012  1.533e-012   -11.815   -11.815
0.000
     BaCl+              1.454e-012  9.849e-013   -11.837   -12.007
-0.169
     TbCl3              1.278e-014  1.278e-014   -13.893   -13.893
0.000
     ZnCl3-             8.791e-015  5.954e-015   -14.056   -14.225
-0.169
     YbCl3              1.013e-015  1.013e-015   -14.995   -14.995
0.000
     ZnCl4-2            1.840e-016  3.318e-017   -15.735   -16.479
-0.744
     MnCl+              1.357e-016  9.191e-017   -15.867   -16.037
-0.169
     UO2Cl+             8.541e-017  5.784e-017   -16.069   -16.238
-0.169
```

```
     TbCl4-            5.096e-018  3.452e-018   -17.293   -17.462
-0.169
     YbCl4-            4.071e-019  2.758e-019   -18.390   -18.559
-0.169
     PuO2Cl+           5.590e-021  3.786e-021   -20.253   -20.422
-0.169
     UO2Cl2            2.177e-021  2.177e-021   -20.662   -20.662
0.000
     FeCl+             8.053e-022  5.454e-022   -21.094   -21.263
-0.169
     FeCl+2            2.232e-022  4.459e-023   -21.651   -22.351
-0.700
     FeCl2+            3.918e-023  2.654e-023   -22.407   -22.576
-0.169
     MnCl3-            1.602e-023  1.085e-023   -22.795   -22.964
-0.169
     FeCl2             2.152e-027  2.152e-027   -26.667   -26.667
0.000
     FeCl4-            2.546e-032  1.725e-032   -31.594   -31.763
-0.169
     FeCl4-2           1.864e-032  3.361e-033   -31.730   -32.474
-0.744
     UCl+3             0.000e+000  0.000e+000   -61.390   -62.902
-1.513
Cl(1)            1.658e-020
     ClO-              1.344e-020  9.105e-021   -19.871   -20.041
-0.169
     HClO              3.134e-021  3.134e-021   -20.504   -20.504
0.000
Cl(3)            2.122e-030
     ClO2-             2.122e-030  1.437e-030   -29.673   -29.842
-0.169
     HClO2             1.972e-035  1.972e-035   -34.705   -34.705
0.000
Cl(5)            2.454e-026
     ClO3-             2.454e-026  1.615e-026   -25.610   -25.792
-0.182
     UO2ClO3+          4.041e-039  2.737e-039   -38.394   -38.563
-0.169
Cl(7)            1.376e-026
     ClO4-             1.376e-026  9.053e-027   -25.861   -26.043
-0.182
     ZnClO4+           3.495e-030  2.367e-030   -29.457   -29.626
-0.169
F                1.277e-003
     AsO3F-2           1.275e-003  2.299e-004    -2.895    -3.639
-0.744
     HAsO3F-           2.339e-006  1.584e-006    -5.631    -5.800
-0.169
     TbF+2             9.274e-014  1.852e-014   -13.033   -13.732
-0.700
```

YbF+2	2.064e-014	4.123e-015	-13.685	-14.385	-0.700
F-	6.974e-015	4.589e-015	-14.157	-14.338	-0.182
NaF	1.023e-016	1.023e-016	-15.990	-15.990	0.000
CaF+	4.284e-017	2.902e-017	-16.368	-16.537	-0.169
MgF+	1.356e-017	9.186e-018	-16.868	-17.037	-0.169
ZnF+	1.323e-018	8.959e-019	-17.878	-18.048	-0.169
HF	6.538e-020	6.538e-020	-19.185	-19.185	0.000
PO3F-2	6.062e-022	1.093e-022	-21.217	-21.961	-0.744
UO2F+	4.224e-023	2.861e-023	-22.374	-22.544	-0.169
BaF+	1.864e-023	1.262e-023	-22.730	-22.899	-0.169
AlF+2	4.639e-024	9.267e-025	-23.334	-24.033	-0.700
VO2F	1.523e-024	1.523e-024	-23.817	-23.817	0.000
TbF2+	4.047e-025	2.741e-025	-24.393	-24.562	-0.169
YbF2+	1.073e-025	7.268e-026	-24.969	-25.139	-0.169
PuO2F+	2.660e-026	1.802e-026	-25.575	-25.744	-0.169
HPO3F-	1.883e-026	1.276e-026	-25.725	-25.894	-0.169
MnF+	1.071e-026	7.251e-027	-25.970	-26.140	-0.169
FeF+2	1.254e-028	2.504e-029	-27.902	-28.601	-0.700
BF2(OH)2-	2.669e-031	1.808e-031	-30.574	-30.743	-0.169
FeF+	1.580e-031	1.070e-031	-30.801	-30.970	-0.169
AlF2+	2.499e-033	1.693e-033	-32.602	-32.771	-0.169
H2PO3F	7.573e-034	7.573e-034	-33.121	-33.121	0.000
UO2F2	3.939e-034	3.939e-034	-33.405	-33.405	0.000
HF2-	1.073e-034	7.267e-035	-33.969	-34.139	-0.169
VOF+	1.935e-035	1.310e-035	-34.713	-34.883	-0.169
PuO2F2	1.634e-035	1.634e-035	-34.787	-34.787	0.000

VO2F2-	2.976e-036	2.015e-036	-35.526	-35.696	-0.169
TbF3	4.609e-037	4.609e-037	-36.336	-36.336	0.000
YbF3	1.656e-037	1.656e-037	-36.781	-36.781	0.000
H2F2	1.063e-038	1.063e-038	-37.973	-37.973	0.000
FeF2+	2.746e-039	1.860e-039	-38.561	-38.731	-0.169
AlF3	0.000e+000	0.000e+000	-43.010	-43.010	0.000
PuF+3	0.000e+000	0.000e+000	-43.844	-45.356	-1.513
PuO2F3-	0.000e+000	0.000e+000	-43.990	-44.160	-0.169
UO2F3-	0.000e+000	0.000e+000	-45.307	-45.476	-0.169
BF3OH-	0.000e+000	0.000e+000	-46.308	-46.477	-0.169
VOF2	0.000e+000	0.000e+000	-46.441	-46.441	0.000
TbF4-	0.000e+000	0.000e+000	-48.430	-48.599	-0.169
YbF4-	0.000e+000	0.000e+000	-48.777	-48.946	-0.169
PuF2+2	0.000e+000	0.000e+000	-52.055	-52.755	-0.700
AlF4-	0.000e+000	0.000e+000	-54.779	-54.948	-0.169
PuO2F4-2	0.000e+000	0.000e+000	-54.880	-55.624	-0.744
UO2F4-2	0.000e+000	0.000e+000	-58.295	-59.039	-0.744
BF4-	0.000e+000	0.000e+000	-63.851	-64.020	-0.169
UF+3	0.000e+000	0.000e+000	-65.050	-66.563	-1.513
UF2+2	0.000e+000	0.000e+000	-73.276	-73.975	-0.700
PuF3+	0.000e+000	0.000e+000	-77.024	-77.193	-0.169
UF3+	0.000e+000	0.000e+000	-82.793	-82.962	-0.169
PuF4	0.000e+000	0.000e+000	-92.631	-92.631	0.000
UF4	0.000e+000	0.000e+000	-93.357	-93.357	0.000
SiF6-2	0.000e+000	0.000e+000	-95.044	-95.788	-0.744
UF5-	0.000e+000	0.000e+000	-106.198	-106.367	-0.169

```
     UF6-2              0.000e+000  0.000e+000  -117.931  -118.675
-0.744
Fe(2)            8.498e-018
     Fe+2               3.985e-018  1.018e-018   -17.400   -17.992
-0.593
     FeSO4              3.929e-018  3.929e-018   -17.406   -17.406
0.000
     FeHCO3+            3.931e-019  2.663e-019   -18.405   -18.575
-0.169
     FeCO3              1.377e-019  1.377e-019   -18.861   -18.861
0.000
     FeOH+              5.049e-020  3.420e-020   -19.297   -19.466
-0.169
     FePO4-             1.051e-021  7.116e-022   -20.979   -21.148
-0.169
     FeCl+              8.053e-022  5.454e-022   -21.094   -21.263
-0.169
     FeHPO4             6.481e-022  6.481e-022   -21.188   -21.188
0.000
     Fe(OH)2            2.885e-023  2.885e-023   -22.540   -22.540
0.000
     Fe(OH)3-           1.801e-025  1.219e-025   -24.745   -24.914
-0.169
     FeCl2              2.152e-027  2.152e-027   -26.667   -26.667
0.000
     FeH2PO4+           1.118e-030  7.572e-031   -29.952   -30.121
-0.169
     FeF+               1.580e-031  1.070e-031   -30.801   -30.970
-0.169
     Fe(OH)4-2          7.183e-032  1.295e-032   -31.144   -31.888
-0.744
     FeCl4-2            1.864e-032  3.361e-033   -31.730   -32.474
-0.744
Fe(3)            4.660e-007
     Fe(OH)3            4.359e-007  4.359e-007    -6.361    -6.361
0.000
     Fe(OH)4-           1.717e-008  1.163e-008    -7.765    -7.935
-0.169
     Fe(OH)2+           1.296e-008  8.775e-009    -7.888    -8.057
-0.169
     FeOH+2             1.249e-012  2.495e-013   -11.903   -12.603
-0.700
     FeCO3+             7.391e-015  5.006e-015   -14.131   -14.301
-0.169
     FeHPO4+            1.300e-015  8.806e-016   -14.886   -15.055
-0.169
     Fe+3               4.034e-018  3.639e-019   -17.394   -18.439
-1.045
     FeSO4+             1.266e-018  8.573e-019   -17.898   -18.067
-0.169
     Fe(SO4)2-          5.210e-019  3.528e-019   -18.283   -18.452
-0.169
```

```
     FeNO3+2            1.491e-020  2.978e-021   -19.827   -20.526
-0.700
     Fe2(OH)2+4         6.156e-022  1.676e-024   -21.211   -23.776
-2.565
     FeCl+2             2.232e-022  4.459e-023   -21.651   -22.351
-0.700
     FeCl2+             3.918e-023  2.654e-023   -22.407   -22.576
-0.169
     Fe3(OH)4+5         2.033e-026  3.073e-030   -25.692   -29.512
-3.821
     FeF+2              1.254e-028  2.504e-029   -27.902   -28.601
-0.700
     FeH2PO4+2          3.999e-029  7.987e-030   -28.398   -29.098
-0.700
     FeNO2+2            7.703e-032  1.539e-032   -31.113   -31.813
-0.700
     FeCl4-             2.546e-032  1.725e-032   -31.594   -31.763
-0.169
     FeF2+              2.746e-039  1.860e-039   -38.561   -38.731
-0.169
H(0)            0.000e+000
     H2                 0.000e+000  0.000e+000   -44.363   -44.308
0.055
I(-03)          0.000e+000
     I3-                0.000e+000  0.000e+000   -48.263   -48.432
-0.169
I(-1)           5.662e-019
     I-                 5.639e-019  3.590e-019   -18.249   -18.445
-0.196
     NaI                2.251e-021  2.251e-021   -20.648   -20.648
0.000
     KI                 1.776e-024  1.776e-024   -23.751   -23.751
0.000
     ZnI+               7.104e-027  4.812e-027   -26.148   -26.318
-0.169
     ZnI2               0.000e+000  0.000e+000   -43.593   -43.593
0.000
     ZnI3-              0.000e+000  0.000e+000   -62.030   -62.200
-0.169
     UI+3               0.000e+000  0.000e+000   -77.203   -78.716
-1.513
     ZnI4-2             0.000e+000  0.000e+000   -80.500   -81.244
-0.744
I(1)            1.033e-021
     IO-                1.033e-021  6.996e-022   -20.986   -21.155
-0.169
I(5)            1.010e-006
     IO3-               1.010e-006  6.841e-007    -5.996    -6.165
-0.169
     HIO3               1.969e-014  1.969e-014   -13.706   -13.706
0.000
```

```
     UO2IO3+          2.825e-018  1.913e-018   -17.549   -17.718
-0.169
     UO2(IO3)2        2.457e-023  2.457e-023   -22.610   -22.610
0.000
I(7)            3.191e-019
     IO4-             3.191e-019  2.100e-019   -18.496   -18.678
-0.182
K               3.562e-004
     K+               3.007e-004  1.914e-004    -3.522    -3.718
-0.196
     KSO4-            5.553e-005  3.761e-005    -4.255    -4.425
-0.169
     KCl              4.725e-009  4.725e-009    -8.326    -8.326
0.000
     KHPO4-           2.722e-010  1.844e-010    -9.565    -9.734
-0.169
     KOH              7.047e-011  7.047e-011   -10.152   -10.152
0.000
     KHSO4            3.080e-013  3.080e-013   -12.511   -12.511
0.000
     KP2O7-3          1.065e-017  2.116e-019   -16.973   -18.675
-1.702
     KI               1.776e-024  1.776e-024   -23.751   -23.751
0.000
Mg              9.261e-004
     MgSO4            5.393e-004  5.393e-004    -3.268    -3.268
0.000
     Mg+2             2.570e-004  8.295e-005    -3.590    -4.081
-0.491
     MgB(OH)4+        1.288e-004  8.725e-005    -3.890    -4.059
-0.169
     MgHCO3+          7.088e-007  4.800e-007    -6.149    -6.319
-0.169
     MgCO3            2.090e-007  2.090e-007    -6.680    -6.680
0.000
     MgCl+            7.030e-008  4.761e-008    -7.153    -7.322
-0.169
     MgHPO4           1.078e-008  1.078e-008    -7.967    -7.967
0.000
     MgPO4-           3.903e-009  2.643e-009    -8.409    -8.578
-0.169
     MgP2O7-2         3.997e-014  7.207e-015   -13.398   -14.142
-0.744
     MgF+             1.356e-017  9.186e-018   -16.868   -17.037
-0.169
     MgH2PO4+         8.307e-018  5.626e-018   -17.081   -17.250
-0.169
     Mg4(OH)4+4       3.934e-022  1.071e-024   -21.405   -23.970
-2.565
Mn(2)           5.887e-013
     MnSO4            3.527e-013  3.527e-013   -12.453   -12.453
0.000
```

```
     Mn+2              2.297e-013  5.871e-014   -12.639   -13.231
-0.593
     MnCO3             4.895e-015  4.895e-015   -14.310   -14.310
0.000
     MnSeO4            5.457e-016  5.457e-016   -15.263   -15.263
0.000
     MnHCO3+           3.288e-016  2.227e-016   -15.483   -15.652
-0.169
     MnOH+             2.366e-016  1.603e-016   -15.626   -15.795
-0.169
     MnCl+             1.357e-016  9.191e-017   -15.867   -16.037
-0.169
     MnNO3+            1.124e-016  7.615e-017   -15.949   -16.118
-0.169
     MnHPO4            3.568e-017  3.568e-017   -16.448   -16.448
0.000
     MnPO4-            1.102e-017  7.465e-018   -16.958   -17.127
-0.169
     Mn(NO3)2          1.565e-019  1.565e-019   -18.805   -18.805
0.000
     MnH2PO4+          4.621e-020  3.130e-020   -19.335   -19.505
-0.169
     Mn(OH)2           4.178e-020  4.178e-020   -19.379   -19.379
0.000
     MnCl3-            1.602e-023  1.085e-023   -22.795   -22.964
-0.169
     Mn(OH)3-          6.144e-024  4.161e-024   -23.212   -23.381
-0.169
     MnF+              1.071e-026  7.251e-027   -25.970   -26.140
-0.169
     Mn2(OH)3+         7.673e-027  5.197e-027   -26.115   -26.284
-0.169
     Mn2OH+3           3.284e-028  1.008e-029   -27.484   -28.996
-1.513
     Mn(OH)4-2         2.076e-029  3.742e-030   -28.683   -29.427
-0.744
Mn(3)            1.901e-025
     Mn+3              1.901e-025  5.837e-027   -24.721   -26.234
-1.513
Mn(6)            3.850e-017
     MnO4-2            3.850e-017  6.942e-018   -16.414   -17.158
-0.744
Mn(7)            1.732e-014
     MnO4-             1.732e-014  1.140e-014   -13.761   -13.943
-0.182
N(-03)           0.000e+000
     N3-               0.000e+000  0.000e+000  -100.039  -100.208
-0.169
     HN3               0.000e+000  0.000e+000  -103.538  -103.538
0.000
     ZnN3+             0.000e+000  0.000e+000  -104.456  -104.625
-0.169
```

```
     UO2N3+            0.000e+000  0.000e+000  -110.736  -110.905
-0.169
     Zn(N3)2           0.000e+000  0.000e+000  -204.080  -204.080
0.000
     UO2(N3)2          0.000e+000  0.000e+000  -209.363  -209.363
0.000
     UO2(N3)3-         0.000e+000  0.000e+000  -307.991  -308.160
-0.169
     UO2(N3)4-2        0.000e+000  0.000e+000  -408.445  -409.189
-0.744
N(-3)            0.000e+000
     NH4+              0.000e+000  0.000e+000   -64.589   -64.801
-0.213
     NH3               0.000e+000  0.000e+000   -66.009   -66.009
0.000
     Zn(NH3)+2         0.000e+000  0.000e+000   -68.116   -68.816
-0.700
     NH4SO4-           0.000e+000  0.000e+000   -74.546   -74.715
-0.169
     Zn(NH3)2+2        0.000e+000  0.000e+000  -131.919  -132.619
-0.700
     Zn(NH3)3+2        0.000e+000  0.000e+000  -195.722  -196.421
-0.700
     SCN-              0.000e+000  0.000e+000  -214.854  -215.036
-0.182
     UO2SCN+           0.000e+000  0.000e+000  -226.733  -226.902
-0.169
     Zn(NH3)4+2        0.000e+000  0.000e+000  -259.798  -260.498
-0.700
     USCN+3            0.000e+000  0.000e+000  -272.031  -273.544
-1.513
     Zn(SCN)2          0.000e+000  0.000e+000  -434.051  -434.051
0.000
     UO2(SCN)2         0.000e+000  0.000e+000  -442.106  -442.106
0.000
     U(SCN)2+2         0.000e+000  0.000e+000  -486.579  -487.279
-0.700
     UO2(SCN)3-        0.000e+000  0.000e+000  -656.113  -656.282
-0.169
     Zn(SCN)4-2        0.000e+000  0.000e+000  -863.011  -863.755
-0.744
N(-5)            0.000e+000
     HCN               0.000e+000  0.000e+000  -122.324  -122.324
0.000
     CN-               0.000e+000  0.000e+000  -123.354  -123.550
-0.196
     Zn(CN)4-2         0.000e+000  0.000e+000  -481.541  -482.285
-0.744
N(0)             2.354e-021
     N2                1.177e-021  1.177e-021   -20.929   -20.929
0.000
N(3)             4.702e-017
```

```
     NO2-              4.702e-017  2.993e-017   -16.328   -16.524
-0.196
     HNO2              4.741e-022  4.741e-022   -21.324   -21.324
0.000
     FeNO2+2           7.703e-032  1.539e-032   -31.113   -31.813
-0.700
N(5)             1.294e-003
     NO3-              1.285e-003  8.183e-004    -2.891    -3.087
-0.196
     CaNO3+            7.534e-006  5.102e-006    -5.123    -5.292
-0.169
     TbNO3+2           1.158e-006  2.312e-007    -5.936    -6.636
-0.700
     YbNO3+2           9.308e-008  1.859e-008    -7.031    -7.731
-0.700
     BaNO3+            3.832e-011  2.596e-011   -10.417   -10.586
-0.169
     HNO3              3.972e-013  3.972e-013   -12.401   -12.401
0.000
     UO2NO3+           1.219e-016  8.256e-017   -15.914   -16.083
-0.169
     MnNO3+            1.124e-016  7.615e-017   -15.949   -16.118
-0.169
     Mn(NO3)2          1.565e-019  1.565e-019   -18.805   -18.805
0.000
     FeNO3+2           1.491e-020  2.978e-021   -19.827   -20.526
-0.700
     UNO3+3            0.000e+000  0.000e+000   -61.610   -63.123
-1.513
     U(NO3)2+2         0.000e+000  0.000e+000   -64.700   -65.399
-0.700
Na               3.625e-001
     Na+               3.076e-001  2.084e-001    -0.512    -0.681
-0.169
     NaSO4-            4.948e-002  3.351e-002    -1.306    -1.475
-0.169
     NaB(OH)4          5.169e-003  5.169e-003    -2.287    -2.287
0.000
     NaHCO3            1.485e-004  1.485e-004    -3.828    -3.828
0.000
     NaCl              2.692e-005  2.692e-005    -4.570    -4.570
0.000
     NaHSiO3           1.117e-005  1.117e-005    -4.952    -4.952
0.000
     NaCO3-            2.564e-006  1.736e-006    -5.591    -5.760
-0.169
     NaHPO4-           4.091e-007  2.771e-007    -6.388    -6.557
-0.169
     NaOH              3.678e-008  3.678e-008    -7.434    -7.434
0.000
     NaAlO2            1.363e-009  1.363e-009    -8.866    -8.866
0.000
```

```
     Na2P2O7-2          1.734e-014  3.127e-015   -13.761   -14.505
-0.744
     NaP2O7-3           9.511e-015  1.889e-016   -14.022   -15.724
-1.702
     NaHP2O7-2          1.968e-015  3.548e-016   -14.706   -15.450
-0.744
     NaF                1.023e-016  1.023e-016   -15.990   -15.990
0.000
     NaI                2.251e-021  2.251e-021   -20.648   -20.648
0.000
O(0)             4.507e-004
     O2                 2.254e-004  2.556e-004    -3.647    -3.592
0.055
     UO2S2O3            0.000e+000  0.000e+000  -156.680  -156.680
0.000
     S3O6-2             0.000e+000  0.000e+000  -175.021  -175.765
-0.744
     S2-2               0.000e+000  0.000e+000  -249.276  -250.020
-0.744
     S4O6-2             0.000e+000  0.000e+000  -266.022  -266.766
-0.744
     S3-2               0.000e+000  0.000e+000  -353.700  -354.444
-0.744
     S5O6-2             0.000e+000  0.000e+000  -385.902  -386.646
-0.744
     S4-2               0.000e+000  0.000e+000  -458.351  -459.095
-0.744
     S5-2               0.000e+000  0.000e+000  -563.218  -563.962
-0.744
P(-3)            0.000e+000
     PH4+               0.000e+000  0.000e+000  -236.280  -236.450
-0.169
P(5)             3.832e-003
     TbPO4              1.700e-003  1.700e-003    -2.770    -2.770
0.000
     YbPO4              8.516e-004  8.516e-004    -3.070    -3.070
0.000
     Yb(PO4)2-3         3.519e-004  6.990e-006    -3.454    -5.156
-1.702
     Tb(PO4)2-3         2.797e-004  5.555e-006    -3.553    -5.255
-1.702
     TbHPO4+            1.228e-005  8.315e-006    -4.911    -5.080
-0.169
     YbHPO4+            3.082e-006  2.088e-006    -5.511    -5.680
-0.169
     HPO4-2             8.866e-007  1.599e-007    -6.052    -6.796
-0.744
     NaHPO4-            4.091e-007  2.771e-007    -6.388    -6.557
-0.169
     CaHPO4             1.093e-007  1.093e-007    -6.961    -6.961
0.000
```

CaPO4-	4.349e-008	2.946e-008	-7.362	-7.531	-0.169
H2PO4-	3.705e-008	2.509e-008	-7.431	-7.600	-0.169
ZnPO4-	1.755e-008	1.188e-008	-7.756	-7.925	-0.169
Tb(HPO4)2-	1.559e-008	1.056e-008	-7.807	-7.976	-0.169
MgHPO4	1.078e-008	1.078e-008	-7.967	-7.967	0.000
Yb(HPO4)2-	7.809e-009	5.289e-009	-8.107	-8.277	-0.169
ZnHPO4	4.021e-009	4.021e-009	-8.396	-8.396	0.000
MgPO4-	3.903e-009	2.643e-009	-8.409	-8.578	-0.169
TbH2PO4+2	1.628e-009	3.252e-010	-8.788	-9.488	-0.700
PO4-3	3.930e-010	7.807e-012	-9.406	-11.108	-1.702
YbH2PO4+2	3.591e-010	7.173e-011	-9.445	-10.144	-0.700
KHPO4-	2.722e-010	1.844e-010	-9.565	-9.734	-0.169
UO2PO4-	1.616e-010	1.095e-010	-9.792	-9.961	-0.169
UO2HPO4	2.327e-012	2.327e-012	-11.633	-11.633	0.000
CaP2O7-2	2.025e-013	3.650e-014	-12.694	-13.438	-0.744
MgP2O7-2	3.997e-014	7.207e-015	-13.398	-14.142	-0.744
H3PO4	3.588e-014	3.588e-014	-13.445	-13.445	0.000
VO2HPO4-	2.366e-014	1.602e-014	-13.626	-13.795	-0.169
Na2P2O7-2	1.734e-014	3.127e-015	-13.761	-14.505	-0.744
NaP2O7-3	9.511e-015	1.889e-016	-14.022	-15.724	-1.702
P2O7-4	5.558e-015	5.033e-018	-14.255	-17.298	-3.043
HP2O7-3	3.839e-015	7.626e-017	-14.416	-16.118	-1.702
NaHP2O7-2	1.968e-015	3.548e-016	-14.706	-15.450	-0.744
FeHPO4+	1.300e-015	8.806e-016	-14.886	-15.055	-0.169
AlHPO4+	1.197e-016	8.109e-017	-15.922	-16.091	-0.169
VO2(HPO4)2-3	7.593e-017	1.508e-018	-16.120	-17.822	-1.702

CaH2PO4+	6.846e-017	4.637e-017	-16.165	-16.334	-0.169
UO2H2PO4+	5.443e-017	3.686e-017	-16.264	-16.433	-0.169
MnHPO4	3.568e-017	3.568e-017	-16.448	-16.448	0.000
H2P2O7-2	1.624e-017	2.927e-018	-16.790	-17.534	-0.744
MnPO4-	1.102e-017	7.465e-018	-16.958	-17.127	-0.169
KP2O7-3	1.065e-017	2.116e-019	-16.973	-18.675	-1.702
MgH2PO4+	8.307e-018	5.626e-018	-17.081	-17.250	-0.169
ZnH2PO4+	8.150e-020	5.520e-020	-19.089	-19.258	-0.169
MnH2PO4+	4.621e-020	3.130e-020	-19.335	-19.505	-0.169
Pu(HPO4)4-4	5.761e-021	5.216e-024	-20.240	-23.283	-3.043
PuO2H2PO4+	3.108e-021	2.105e-021	-20.507	-20.677	-0.169
FePO4-	1.051e-021	7.116e-022	-20.979	-21.148	-0.169
FeHPO4	6.481e-022	6.481e-022	-21.188	-21.188	0.000
UO2(H2PO4)2	6.453e-022	6.453e-022	-21.190	-21.190	0.000
PO3F-2	6.062e-022	1.093e-022	-21.217	-21.961	-0.744
H3P2O7-	9.220e-024	6.245e-024	-23.035	-23.204	-0.169
UO2H3PO4+2	7.477e-025	1.493e-025	-24.126	-24.826	-0.700
Pu(HPO4)3-2	2.646e-026	4.771e-027	-25.577	-26.321	-0.744
HPO3F-	1.883e-026	1.276e-026	-25.725	-25.894	-0.169
VO2H2PO4	1.053e-026	1.053e-026	-25.978	-25.978	0.000
AlH2PO4+2	1.889e-028	3.772e-029	-27.724	-28.423	-0.700
UO2(H2PO4)(H3PO4)+	9.049e-029	6.129e-029	-28.043	-28.213	-0.169
FeH2PO4+2	3.999e-029	7.987e-030	-28.398	-29.098	-0.700
Pu(HPO4)2	6.557e-030	6.557e-030	-29.183	-29.183	0.000
H4P2O7	1.703e-030	1.703e-030	-29.769	-29.769	0.000
FeH2PO4+	1.118e-030	7.572e-031	-29.952	-30.121	-0.169

```
     PuHPO4+2          2.969e-033  5.930e-034   -32.527   -33.227
-0.700
     H2PO3F            7.573e-034  7.573e-034   -33.121   -33.121
0.000
     PuH2PO4+2         3.473e-040  0.000e+000   -39.459   -40.159
-0.700
Pu(3)            1.752e-032
     Pu(SO4)2-         1.612e-032  1.092e-032   -31.793   -31.962
-0.169
     PuSO4+            1.062e-033  7.192e-034   -32.974   -33.143
-0.169
     Pu+3              2.872e-034  8.817e-036   -33.542   -35.055
-1.513
     PuOH+2            5.023e-035  1.003e-035   -34.299   -34.999
-0.700
     PuH2PO4+2         3.473e-040  0.000e+000   -39.459   -40.159
-0.700
Pu(4)            1.376e-017
     Pu(OH)4           1.375e-017  1.375e-017   -16.862   -16.862
0.000
     Pu(HPO4)4-4       5.761e-021  5.216e-024   -20.240   -23.283
-3.043
     Pu(OH)3+          3.020e-021  2.046e-021   -20.520   -20.689
-0.169
     Pu(OH)2+2         8.892e-026  1.776e-026   -25.051   -25.751
-0.700
     Pu(HPO4)3-2       2.646e-026  4.771e-027   -25.577   -26.321
-0.744
     Pu(HPO4)2         6.557e-030  6.557e-030   -29.183   -29.183
0.000
     PuOH+3            3.603e-031  1.106e-032   -30.443   -31.956
-1.513
     Pu(SO4)2          3.730e-033  3.730e-033   -32.428   -32.428
0.000
     PuHPO4+2          2.969e-033  5.930e-034   -32.527   -33.227
-0.700
     PuSO4+2           2.597e-035  5.186e-036   -34.586   -35.285
-0.700
     Pu+4              1.221e-037  3.325e-040   -36.913   -39.478
-2.565
     PuF+3             0.000e+000  0.000e+000   -43.844   -45.356
-1.513
     PuF2+2            0.000e+000  0.000e+000   -52.055   -52.755
-0.700
     PuF3+             0.000e+000  0.000e+000   -77.024   -77.193
-0.169
     PuF4              0.000e+000  0.000e+000   -92.631   -92.631
0.000
Pu(5)            6.586e-014
     PuO2+             6.484e-014  4.391e-014   -13.188   -13.357
-0.169
```

```
      PuO2OH              1.021e-015  1.021e-015   -14.991   -14.991
0.000
Pu(6)             2.429e-013
      PuO2(CO3)2-2        2.396e-013  4.320e-014   -12.621   -13.365
-0.744
      PuO2OH+             2.901e-015  1.965e-015   -14.537   -14.707
-0.169
      PuO2SO4             3.719e-016  3.719e-016   -15.430   -15.430
0.000
      PuO2+2              4.036e-017  8.061e-018   -16.394   -17.094
-0.700
      PuO2Cl+             5.590e-021  3.786e-021   -20.253   -20.422
-0.169
      PuO2H2PO4+          3.108e-021  2.105e-021   -20.507   -20.677
-0.169
      PuO2F+              2.660e-026  1.802e-026   -25.575   -25.744
-0.169
      (PuO2)2(OH)2+2      2.011e-026  4.017e-027   -25.697   -26.396
-0.700
      (PuO2)3(OH)5+       2.296e-033  1.555e-033   -32.639   -32.808
-0.169
      PuO2F2              1.634e-035  1.634e-035   -34.787   -34.787
0.000
      PuO2F3-             0.000e+000  0.000e+000   -43.990   -44.160
-0.169
      PuO2F4-2            0.000e+000  0.000e+000   -54.880   -55.624
-0.744
S(-2)             0.000e+000
      HS-                 0.000e+000  0.000e+000  -140.562  -140.744
-0.182
      H2S                 0.000e+000  0.000e+000  -141.767  -141.767
0.000
      S-2                 0.000e+000  0.000e+000  -144.977  -145.637
-0.660
      SCN-                0.000e+000  0.000e+000  -214.854  -215.036
-0.182
      UO2SCN+             0.000e+000  0.000e+000  -226.733  -226.902
-0.169
      S2-2                0.000e+000  0.000e+000  -249.276  -250.020
-0.744
      USCN+3              0.000e+000  0.000e+000  -272.031  -273.544
-1.513
      HAsS2               0.000e+000  0.000e+000  -333.373  -333.373
0.000
      S3-2                0.000e+000  0.000e+000  -353.700  -354.444
-0.744
      Zn(SCN)2            0.000e+000  0.000e+000  -434.051  -434.051
0.000
      UO2(SCN)2           0.000e+000  0.000e+000  -442.106  -442.106
0.000
      S4-2                0.000e+000  0.000e+000  -458.351  -459.095
-0.744
```

```
     U(SCN)2+2          0.000e+000  0.000e+000  -486.579  -487.279
-0.700
     S5-2               0.000e+000  0.000e+000  -563.218  -563.962
-0.744
     UO2(SCN)3-         0.000e+000  0.000e+000  -656.113  -656.282
-0.169
     Zn(SCN)4-2         0.000e+000  0.000e+000  -863.011  -863.755
-0.744
S(2)             0.000e+000
     S2O3-2             0.000e+000  0.000e+000  -144.831  -145.575
-0.744
     HS2O3-             0.000e+000  0.000e+000  -152.424  -152.593
-0.169
S(3)             0.000e+000
     S2O4-2             0.000e+000  0.000e+000  -134.136  -134.795
-0.660
S(4)             0.000e+000
     SO3-2              0.000e+000  0.000e+000   -45.736   -46.435
-0.700
     HSO3-              0.000e+000  0.000e+000   -47.067   -47.236
-0.169
     UO2SO3             0.000e+000  0.000e+000   -52.959   -52.959
0.000
     H2SO3              0.000e+000  0.000e+000   -53.287   -53.287
0.000
     SO2                0.000e+000  0.000e+000   -53.381   -53.381
0.000
     UO2(SO3)2-2        0.000e+000  0.000e+000   -97.493   -98.237
-0.744
     S2O5-2             0.000e+000  0.000e+000   -98.552   -99.296
-0.744
     UO2S2O3            0.000e+000  0.000e+000  -156.680  -156.680
0.000
     S3O6-2             0.000e+000  0.000e+000  -175.021  -175.765
-0.744
     S4O6-2             0.000e+000  0.000e+000  -266.022  -266.766
-0.744
     S5O6-2             0.000e+000  0.000e+000  -385.902  -386.646
-0.744
S(5)             0.000e+000
     S2O6-2             0.000e+000  0.000e+000   -68.114   -68.858
-0.744
S(6)             2.235e-001
     SO4-2              1.350e-001  2.435e-002    -0.870    -1.614
-0.744
     NaSO4-             4.948e-002  3.351e-002    -1.306    -1.475
-0.169
     TbSO4+             1.463e-002  9.907e-003    -1.835    -2.004
-0.169
     Tb(SO4)2-          7.214e-003  4.886e-003    -2.142    -2.311
-0.169
```

CaSO4	4.424e-003	4.424e-003	-2.354	-2.354	0.000
YbSO4+	1.960e-003	1.328e-003	-2.708	-2.877	-0.169
Yb(SO4)2-	1.439e-003	9.744e-004	-2.842	-3.011	-0.169
MgSO4	5.393e-004	5.393e-004	-3.268	-3.268	0.000
ZnSO4	7.071e-005	7.071e-005	-4.151	-4.151	0.000
KSO4-	5.553e-005	3.761e-005	-4.255	-4.425	-0.169
HSO4-	3.370e-008	2.282e-008	-7.472	-7.642	-0.169
UO2(SO4)2-2	1.873e-012	3.377e-013	-11.727	-12.471	-0.744
UO2SO4	1.565e-012	1.565e-012	-11.805	-11.805	0.000
MnSO4	3.527e-013	3.527e-013	-12.453	-12.453	0.000
KHSO4	3.080e-013	3.080e-013	-12.511	-12.511	0.000
VO2SO4-	2.026e-013	1.372e-013	-12.693	-12.863	-0.169
Al(SO4)2-	1.404e-015	9.508e-016	-14.853	-15.022	-0.169
AlSO4+	7.428e-016	5.031e-016	-15.129	-15.298	-0.169
PuO2SO4	3.719e-016	3.719e-016	-15.430	-15.430	0.000
FeSO4	3.929e-018	3.929e-018	-17.406	-17.406	0.000
FeSO4+	1.266e-018	8.573e-019	-17.898	-18.067	-0.169
Fe(SO4)2-	5.210e-019	3.528e-019	-18.283	-18.452	-0.169
H2SO4	1.999e-019	1.999e-019	-18.699	-18.699	0.000
VOSO4	2.099e-024	2.099e-024	-23.678	-23.678	0.000
Pu(SO4)2-	1.612e-032	1.092e-032	-31.793	-31.962	-0.169
Pu(SO4)2	3.730e-033	3.730e-033	-32.428	-32.428	0.000
PuSO4+	1.062e-033	7.192e-034	-32.974	-33.143	-0.169
PuSO4+2	2.597e-035	5.186e-036	-34.586	-35.285	-0.700
VSO4+	0.000e+000	0.000e+000	-45.493	-45.662	-0.169
U(SO4)2	0.000e+000	0.000e+000	-54.339	-54.339	0.000

```
     USO4+2            0.000e+000  0.000e+000   -55.866   -56.565
-0.700
     NH4SO4-           0.000e+000  0.000e+000   -74.546   -74.715
-0.169
S(7)            0.000e+000
     S2O8-2            0.000e+000  0.000e+000   -42.793   -43.537
-0.744
S(8)            2.927e-029
     HSO5-             2.927e-029  1.982e-029   -28.534   -28.703
-0.169
Se(-2)          0.000e+000
     HSe-              0.000e+000  0.000e+000   -95.931   -96.100
-0.169
     H2Se              0.000e+000  0.000e+000  -100.311  -100.311
0.000
     Se-2              0.000e+000  0.000e+000  -102.270  -103.014
-0.744
Se(4)           1.314e-016
     SeO3-2            1.251e-016  2.255e-017   -15.903   -16.647
-0.744
     HSeO3-            6.352e-018  4.302e-018   -17.197   -17.366
-0.169
     H2SeO3            1.517e-023  1.517e-023   -22.819   -22.819
0.000
Se(6)           1.916e-004
     SeO4-2            1.915e-004  3.453e-005    -3.718    -4.462
-0.744
     ZnSeO4            7.393e-008  7.393e-008    -7.131    -7.131
0.000
     HSeO4-            4.024e-011  2.726e-011   -10.395   -10.565
-0.169
     MnSeO4            5.457e-016  5.457e-016   -15.263   -15.263
0.000
Si              1.066e-004
     SiO2              9.379e-005  9.379e-005    -4.028    -4.028
0.000
     NaHSiO3           1.117e-005  1.117e-005    -4.952    -4.952
0.000
     HSiO3-            1.680e-006  1.138e-006    -5.775    -5.944
-0.169
     H2SiO4-2          6.432e-011  1.160e-011   -10.192   -10.936
-0.744
     H6(H2SiO4)4-2     1.016e-013  1.833e-014   -12.993   -13.737
-0.744
     H4(H2SiO4)4-4     1.177e-017  1.066e-020   -16.929   -19.972
-3.043
     SiF6-2            0.000e+000  0.000e+000   -95.044   -95.788
-0.744
Tb(2)           0.000e+000
     Tb+2              0.000e+000  0.000e+000   -73.232   -73.932
-0.700
Tb(3)           6.386e-002
```

```
     TbCO3+            2.687e-002  1.820e-002    -1.571    -1.740
-0.169
     TbSO4+            1.463e-002  9.907e-003    -1.835    -2.004
-0.169
     Tb(CO3)2-         9.715e-003  6.580e-003    -2.013    -2.182
-0.169
     Tb(SO4)2-         7.214e-003  4.886e-003    -2.142    -2.311
-0.169
     Tb+3              2.685e-003  8.244e-005    -2.571    -4.084
-1.513
     TbPO4             1.700e-003  1.700e-003    -2.770    -2.770
0.000
     TbOH+2            6.497e-004  1.298e-004    -3.187    -3.887
-0.700
     Tb(PO4)2-3        2.797e-004  5.555e-006    -3.553    -5.255
-1.702
     TbO+              9.052e-005  6.131e-005    -4.043    -4.212
-0.169
     TbHPO4+           1.228e-005  8.315e-006    -4.911    -5.080
-0.169
     TbHCO3+2          1.097e-005  2.191e-006    -4.960    -5.659
-0.700
     TbO2H             8.678e-006  8.678e-006    -5.062    -5.062
0.000
     TbNO3+2           1.158e-006  2.312e-007    -5.936    -6.636
-0.700
     TbO2-             9.493e-007  6.429e-007    -6.023    -6.192
-0.169
     TbCl+2            5.515e-007  1.102e-007    -6.258    -6.958
-0.700
     Tb(HPO4)2-        1.559e-008  1.056e-008    -7.807    -7.976
-0.169
     TbH2PO4+2         1.628e-009  3.252e-010    -8.788    -9.488
-0.700
     TbCl2+            6.547e-011  4.434e-011   -10.184   -10.353
-0.169
     TbF+2             9.274e-014  1.852e-014   -13.033   -13.732
-0.700
     TbCl3             1.278e-014  1.278e-014   -13.893   -13.893
0.000
     TbCl4-            5.096e-018  3.452e-018   -17.293   -17.462
-0.169
     TbF2+             4.047e-025  2.741e-025   -24.393   -24.562
-0.169
     TbF3              4.609e-037  4.609e-037   -36.336   -36.336
0.000
     TbF4-             0.000e+000  0.000e+000   -48.430   -48.599
-0.169
Tc(3)          0.000e+000
     Tc+3              0.000e+000  0.000e+000   -82.011   -83.523
-1.513
Tc(4)          0.000e+000
```

```
     TcO(OH)2          0.000e+000  0.000e+000   -47.554   -47.554
0.000
     TcOOH+            0.000e+000  0.000e+000   -53.224   -53.394
-0.169
     TcO+2             0.000e+000  0.000e+000   -59.585   -60.284
-0.700
     (TcO(OH)2)2       0.000e+000  0.000e+000   -88.591   -88.591
0.000
Tc(5)            0.000e+000
     TcO4-3            0.000e+000  0.000e+000   -51.117   -52.819
-1.702
Tc(6)            6.619e-030
     HTcO4-            3.688e-030  2.498e-030   -29.433   -29.602
-0.169
     TcO4-2            2.930e-030  5.283e-031   -29.533   -30.277
-0.744
     H2TcO4            4.603e-038  4.603e-038   -37.337   -37.337
0.000
Tc(7)            6.088e-008
     TcO4-             6.088e-008  4.123e-008    -7.216    -7.385
-0.169
U(3)             0.000e+000
     U+3               0.000e+000  0.000e+000   -81.895   -83.408
-1.513
U(4)             1.199e-034
     U(OH)4            1.199e-034  1.199e-034   -33.921   -33.921
0.000
     U(CO3)4-4         0.000e+000  0.000e+000   -45.777   -48.820
-3.043
     U(CO3)5-6         0.000e+000  0.000e+000   -48.651   -55.526
-6.875
     UOH+3             0.000e+000  0.000e+000   -52.493   -54.006
-1.513
     U(SO4)2           0.000e+000  0.000e+000   -54.339   -54.339
0.000
     USO4+2            0.000e+000  0.000e+000   -55.866   -56.565
-0.700
     U+4               0.000e+000  0.000e+000   -58.921   -61.486
-2.565
     UCl+3             0.000e+000  0.000e+000   -61.390   -62.902
-1.513
     UNO3+3            0.000e+000  0.000e+000   -61.610   -63.123
-1.513
     U(NO3)2+2         0.000e+000  0.000e+000   -64.700   -65.399
-0.700
     UF+3              0.000e+000  0.000e+000   -65.050   -66.563
-1.513
     UF2+2             0.000e+000  0.000e+000   -73.276   -73.975
-0.700
     UI+3              0.000e+000  0.000e+000   -77.203   -78.716
-1.513
```

```
     UF3+                0.000e+000  0.000e+000   -82.793   -82.962
-0.169
     UF4                 0.000e+000  0.000e+000   -93.357   -93.357
0.000
     UF5-                0.000e+000  0.000e+000  -106.198  -106.367
-0.169
     UF6-2               0.000e+000  0.000e+000  -117.931  -118.675
-0.744
     USCN+3              0.000e+000  0.000e+000  -272.031  -273.544
-1.513
     U(SCN)2+2           0.000e+000  0.000e+000  -486.579  -487.279
-0.700
U(5)             6.337e-025
     UO2+                6.337e-025  4.292e-025   -24.198   -24.367
-0.169
     UO2(CO3)3-5         9.236e-030  1.578e-034   -29.035   -33.802
-4.767
U(6)             3.625e-006
     UO2(CO3)3-4         3.426e-006  3.103e-009    -5.465    -8.508
-3.043
     UO2(CO3)2-2         1.606e-007  2.895e-008    -6.794    -7.538
-0.744
     UO2(OH)2            2.890e-008  2.890e-008    -7.539    -7.539
0.000
     UO2(OH)3-           5.611e-009  3.800e-009    -8.251    -8.420
-0.169
     (UO2)2CO3(OH)3-     1.589e-009  1.076e-009    -8.799    -8.968
-0.169
     UO2CO3              6.320e-010  6.320e-010    -9.199    -9.199
0.000
     UO2PO4-             1.616e-010  1.095e-010    -9.792    -9.961
-0.169
     UO2OH+              5.132e-011  3.476e-011   -10.290   -10.459
-0.169
     UO2HPO4             2.327e-012  2.327e-012   -11.633   -11.633
0.000
     UO2(SO4)2-2         1.873e-012  3.377e-013   -11.727   -12.471
-0.744
     UO2SO4              1.565e-012  1.565e-012   -11.805   -11.805
0.000
     UO2+2               2.648e-013  5.288e-014   -12.577   -13.277
-0.700
     (UO2)3(CO3)6-6      2.591e-013  3.456e-020   -12.587   -19.461
-6.875
     UO2(OH)4-2          3.489e-014  6.290e-015   -13.457   -14.201
-0.744
     (UO2)3(OH)7-        2.959e-015  2.004e-015   -14.529   -14.698
-0.169
     (UO2)3(OH)5+        7.514e-016  5.089e-016   -15.124   -15.293
-0.169
     (UO2)2(OH)2+2       3.671e-016  7.333e-017   -15.435   -16.135
-0.700
```

```
     UO2NO3+            1.219e-016  8.256e-017   -15.914   -16.083
-0.169
     UO2Cl+             8.541e-017  5.784e-017   -16.069   -16.238
-0.169
     UO2H2PO4+          5.443e-017  3.686e-017   -16.264   -16.433
-0.169
     UO2IO3+            2.825e-018  1.913e-018   -17.549   -17.718
-0.169
     (UO2)4(OH)7+       1.970e-019  1.334e-019   -18.706   -18.875
-0.169
     (UO2)3(OH)4+2      1.109e-019  2.215e-020   -18.955   -19.655
-0.700
     (UO2)2OH+3         1.898e-020  5.829e-022   -19.722   -21.234
-1.513
     (UO2)3(OH)5CO2+    3.324e-021  2.251e-021   -20.478   -20.648
-0.169
     (UO2)3O(OH)2(HCO3)+  2.719e-021  1.842e-021   -20.566   -
20.735    -0.169
     UO2Cl2             2.177e-021  2.177e-021   -20.662   -20.662
0.000
     UO2(H2PO4)2        6.453e-022  6.453e-022   -21.190   -21.190
0.000
     UO2F+              4.224e-023  2.861e-023   -22.374   -22.544
-0.169
     UO2(IO3)2          2.457e-023  2.457e-023   -22.610   -22.610
0.000
     UO2H3PO4+2         7.477e-025  1.493e-025   -24.126   -24.826
-0.700
     UO2(H2PO4)(H3PO4)+  9.049e-029  6.129e-029   -28.043   -28.213
-0.169
     UO2F2              3.939e-034  3.939e-034   -33.405   -33.405
0.000
     UO2ClO3+           4.041e-039  2.737e-039   -38.394   -38.563
-0.169
     UO2F3-             0.000e+000  0.000e+000   -45.307   -45.476
-0.169
     (UO2)11(CO3)6(OH)12-2  0.000e+000  0.000e+000   -46.342   -
47.086    -0.744
     UO2SO3             0.000e+000  0.000e+000   -52.959   -52.959
0.000
     UO2F4-2            0.000e+000  0.000e+000   -58.295   -59.039
-0.744
     UO2(SO3)2-2        0.000e+000  0.000e+000   -97.493   -98.237
-0.744
     UO2N3+             0.000e+000  0.000e+000  -110.736  -110.905
-0.169
     UO2S2O3            0.000e+000  0.000e+000  -156.680  -156.680
0.000
     UO2(N3)2           0.000e+000  0.000e+000  -209.363  -209.363
0.000
     UO2SCN+            0.000e+000  0.000e+000  -226.733  -226.902
-0.169
```

```
     UO2(N3)3-          0.000e+000  0.000e+000  -307.991  -308.160
-0.169
     UO2(N3)4-2         0.000e+000  0.000e+000  -408.445  -409.189
-0.744
     UO2(SCN)2          0.000e+000  0.000e+000  -442.106  -442.106
0.000
     UO2(SCN)3-         0.000e+000  0.000e+000  -656.113  -656.282
-0.169
V(3)             8.393e-038
     V(OH)2+            8.393e-038  5.685e-038   -37.076   -37.245
-0.169
     VOH+2              0.000e+000  0.000e+000   -40.913   -41.612
-0.700
     VSO4+              0.000e+000  0.000e+000   -45.493   -45.662
-0.169
     V+3                0.000e+000  0.000e+000   -45.865   -47.378
-1.513
     V2(OH)2+4          0.000e+000  0.000e+000   -79.939   -82.504
-2.565
V(4)             9.925e-023
     VOOH+              9.572e-023  6.483e-023   -22.019   -22.188
-0.169
     VOSO4              2.099e-024  2.099e-024   -23.678   -23.678
0.000
     VO+2               1.430e-024  2.855e-025   -23.845   -24.544
-0.700
     VOF+               1.935e-035  1.310e-035   -34.713   -34.883
-0.169
     (VO)2(OH)2+2       9.842e-040  1.966e-040   -39.007   -39.706
-0.700
     VOF2               0.000e+000  0.000e+000   -46.441   -46.441
0.000
V(5)             7.451e-003
     VO3OH-2            6.487e-003  1.170e-003    -2.188    -2.932
-0.744
     HVO4-2             6.458e-004  1.164e-004    -3.190    -3.934
-0.744
     H2VO4-             1.937e-004  1.312e-004    -3.713    -3.882
-0.169
     VO2(OH)2-          1.237e-004  8.379e-005    -3.908    -4.077
-0.169
     VO4-3              3.487e-008  6.926e-010    -7.458    -9.160
-1.702
     VO(OH)3            7.777e-009  7.777e-009    -8.109    -8.109
0.000
     VO2+               2.189e-013  1.482e-013   -12.660   -12.829
-0.169
     VO2SO4-            2.026e-013  1.372e-013   -12.693   -12.863
-0.169
     VO2HPO4-           2.366e-014  1.602e-014   -13.626   -13.795
-0.169
```

```
     VO2(HPO4)2-3      7.593e-017  1.508e-018   -16.120   -17.822
-1.702
     VO2F              1.523e-024  1.523e-024   -23.817   -23.817
0.000
     VO2H2PO4          1.053e-026  1.053e-026   -25.978   -25.978
0.000
     VO2F2-            2.976e-036  2.015e-036   -35.526   -35.696
-0.169
Yb(2)            1.960e-035
     Yb+2              1.960e-035  3.915e-036   -34.708   -35.407
-0.700
Yb(3)            2.001e-002
     YbCO3+            9.875e-003  6.688e-003    -2.005    -2.175
-0.169
     Yb(CO3)2-         4.866e-003  3.296e-003    -2.313    -2.482
-0.169
     YbSO4+            1.960e-003  1.328e-003    -2.708    -2.877
-0.169
     Yb(SO4)2-         1.439e-003  9.744e-004    -2.842    -3.011
-0.169
     YbPO4             8.516e-004  8.516e-004    -3.070    -3.070
0.000
     Yb+3              4.253e-004  1.306e-005    -3.371    -4.884
-1.513
     Yb(PO4)2-3        3.519e-004  6.990e-006    -3.454    -5.156
-1.702
     YbOH+2            1.706e-004  3.408e-005    -3.768    -4.467
-0.700
     YbO+              3.912e-005  2.650e-005    -4.408    -4.577
-0.169
     YbO2H             2.083e-005  2.083e-005    -4.681    -4.681
0.000
     YbO2-             5.188e-006  3.514e-006    -5.285    -5.454
-0.169
     YbHPO4+           3.082e-006  2.088e-006    -5.511    -5.680
-0.169
     YbHCO3+2          2.413e-006  4.819e-007    -5.617    -6.317
-0.700
     YbNO3+2           9.308e-008  1.859e-008    -7.031    -7.731
-0.700
     YbCl+2            7.390e-008  1.476e-008    -7.131    -7.831
-0.700
     Yb(HPO4)2-        7.809e-009  5.289e-009    -8.107    -8.277
-0.169
     YbH2PO4+2         3.591e-010  7.173e-011    -9.445   -10.144
-0.700
     YbCl2+            6.349e-012  4.300e-012   -11.197   -11.367
-0.169
     YbF+2             2.064e-014  4.123e-015   -13.685   -14.385
-0.700
     YbCl3             1.013e-015  1.013e-015   -14.995   -14.995
0.000
```

```
     YbCl4-            4.071e-019  2.758e-019   -18.390   -18.559
-0.169
     YbF2+             1.073e-025  7.268e-026   -24.969   -25.139
-0.169
     YbF3              1.656e-037  1.656e-037   -36.781   -36.781
0.000
     YbF4-             0.000e+000  0.000e+000   -48.777   -48.946
-0.169
Zn                1.286e-004
     ZnSO4             7.071e-005  7.071e-005    -4.151    -4.151
0.000
     Zn+2              5.409e-005  1.382e-005    -4.267    -4.859
-0.593
     ZnOH+             2.377e-006  1.610e-006    -5.624    -5.793
-0.169
     Zn(OH)2           7.322e-007  7.322e-007    -6.135    -6.135
0.000
     ZnCO3             2.765e-007  2.765e-007    -6.558    -6.558
0.000
     ZnHCO3+           2.621e-007  1.775e-007    -6.582    -6.751
-0.169
     ZnSeO4            7.393e-008  7.393e-008    -7.131    -7.131
0.000
     Zn(OH)Cl          3.100e-008  3.100e-008    -7.509    -7.509
0.000
     ZnCl+             2.521e-008  1.707e-008    -7.598    -7.768
-0.169
     ZnPO4-            1.755e-008  1.188e-008    -7.756    -7.925
-0.169
     ZnHPO4            4.021e-009  4.021e-009    -8.396    -8.396
0.000
     Zn(OH)3-          3.558e-010  2.410e-010    -9.449    -9.618
-0.169
     ZnCl2             1.466e-011  1.466e-011   -10.834   -10.834
0.000
     Zn(OH)4-2         2.420e-014  4.363e-015   -13.616   -14.360
-0.744
     ZnCl3-            8.791e-015  5.954e-015   -14.056   -14.225
-0.169
     ZnCl4-2           1.840e-016  3.318e-017   -15.735   -16.479
-0.744
     ZnF+              1.323e-018  8.959e-019   -17.878   -18.048
-0.169
     ZnH2PO4+          8.150e-020  5.520e-020   -19.089   -19.258
-0.169
     ZnI+              7.104e-027  4.812e-027   -26.148   -26.318
-0.169
     ZnClO4+           3.495e-030  2.367e-030   -29.457   -29.626
-0.169
     ZnI2              0.000e+000  0.000e+000   -43.593   -43.593
0.000
```

```
     ZnI3-              0.000e+000  0.000e+000   -62.030   -62.200
-0.169
     Zn(NH3)+2          0.000e+000  0.000e+000   -68.116   -68.816
-0.700
     ZnI4-2             0.000e+000  0.000e+000   -80.500   -81.244
-0.744
     ZnN3+              0.000e+000  0.000e+000  -104.456  -104.625
-0.169
     Zn(NH3)2+2         0.000e+000  0.000e+000  -131.919  -132.619
-0.700
     Zn(NH3)3+2         0.000e+000  0.000e+000  -195.722  -196.421
-0.700
     Zn(N3)2            0.000e+000  0.000e+000  -204.080  -204.080
0.000
     Zn(NH3)4+2         0.000e+000  0.000e+000  -259.798  -260.498
-0.700
     Zn(SCN)2           0.000e+000  0.000e+000  -434.051  -434.051
0.000
     Zn(CN)4-2          0.000e+000  0.000e+000  -481.541  -482.285
-0.744
     Zn(SCN)4-2         0.000e+000  0.000e+000  -863.011  -863.755
-0.744

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

     Phase                SI log IAP  log KT

     (UO2)2As2O7      -77.27  -69.59    7.68  (UO2)2As2O7
     (UO2)2Cl3        -59.72  -48.53   11.20  (UO2)2Cl3
     (UO2)2P2O7       -25.37  -40.14  -14.77  (UO2)2P2O7
     (UO2)3(AsO4)2    -76.10  -66.80    9.29  (UO2)3(AsO4)2
     (UO2)3(PO4)2     -23.26  -37.36  -14.10  (UO2)3(PO4)2
     (UO2)3(PO4)2:4H2O -10.33  -37.38  -27.05  (UO2)3(PO4)2:4H2O
     (VO)3(PO4)2     -119.95 -121.90   -1.96  (VO)3(PO4)2
     Afwillite        -28.58   31.39   59.96  Ca3Si2O4(OH)6
     Akermanite       -15.00   30.23   45.23  Ca2MgSi2O7
     Al              -139.83  -54.41   85.42  Al
     Al(g)           -190.53  -54.41  136.12  Al
     Al2(SO4)3        -57.13  -38.23   18.90  Al2(SO4)3
     Al2(SO4)3:6H2O   -39.82  -38.27    1.56  Al2(SO4)3:6H2O
     Alabandite      -145.52 -179.65  -34.13  MnS
     Albite             0.00    2.66    2.66  NaAlSi3O8
     Albite_high       -1.32    2.66    3.98  NaAlSi3O8
     Albite_low        -0.00    2.66    2.66  NaAlSi3O8
     AlF3             -42.44  -59.71  -17.27  AlF3
     Alstonite         -4.43   -1.84    2.58  BaCa(CO3)2
     Alum-K           -18.74  -23.72   -4.97  KAl(SO4)2:12H2O
     Alunite           -8.40   -8.87   -0.47  KAl3(OH)6(SO4)2
     Amesite-14A       -5.87   69.40   75.27  Mg4Al4Si2O10(OH)8
     Analcime          -0.13    5.93    6.06  Na.96Al.96Si2.04O6:H2O
     Analcime-dehy     -6.49    5.93   12.42  Na.96Al.96Si2.04O6
```

Andalusite	-5.12	10.76	15.88	Al2SiO5
Andradite	5.49	64.71	59.22	Ca3Fe2(SiO4)3
Anhydrite	-0.17	-4.52	-4.35	CaSO4
Annite	-35.52	-6.19	29.33	KFe3AlSi3O10(OH)2
Anorthite	-6.59	19.88	26.48	CaAl2(SiO4)2
Antarcticite	-13.30	-9.21	4.09	CaCl2:6H2O
Anthophyllite	-14.87	51.61	66.48	Mg7Si8O22(OH)2
Antigorite	-37.86	437.77	475.63	Mg48Si34O85(OH)62
Aphthitalite	-11.17	-15.06	-3.89	NaK3(SO4)2
Aragonite	-0.15	1.82	1.97	CaCO3
Arcanite	-7.21	-9.05	-1.84	K2SO4
Arsenolite	-112.78	-157.55	-44.77	As2O3
Arsenopyrite	-262.21	-324.99	-62.78	FeAsS
Artinite	-7.03	12.60	19.63	Mg2CO3(OH)2:3H2O
As	-106.30	-140.58	-34.28	As
As2O5	-77.28	-75.15	2.14	As2O5
As4O6(cubi)	-225.42	-315.10	-89.69	As4O6
As4O6(mono)	-225.19	-315.10	-89.91	As4O6
Autunite-H	-14.79	-40.15	-25.35	H2(UO2)2(PO4)2
B	-107.51	-62.45	45.06	B
B(g)	-198.80	-62.45	136.35	B
B2O3	-6.84	-1.30	5.55	B2O3
Ba	-131.77	-33.54	98.23	Ba
Ba(OH)2:8H2O	-16.89	7.60	24.49	Ba(OH)2:8H2O
Ba2Si3O8	-19.99	3.24	23.23	Ba2Si3O8
Ba2SiO4	-33.26	11.29	44.55	Ba2SiO4
Ba2U2O7	-53.81	-20.32	33.49	Ba2U2O7
Ba3UO6	-68.60	25.76	94.36	Ba3UO6
BaCl2	-16.89	-14.67	2.23	BaCl2
BaCl2:2H2O	-14.89	-14.68	0.21	BaCl2:2H2O
BaCl2:H2O	-15.50	-14.67	0.82	BaCl2:H2O
BaHPO4	-7.79	-15.19	-7.40	BaHPO4
BaI2	-56.33	-267.94	-211.61	BaI2
BaMnO4	-15.47	92.89	108.36	BaMnO4
BaO	-40.14	7.66	47.80	BaO
Barite	0.00	-10.01	-10.01	BaSO4
Barytocalcite	-4.59	-1.84	2.74	BaCa(CO3)2
BaS	-157.35	-174.82	-17.47	BaS
BaSeO3	-18.47	-54.06	-35.59	BaSeO3
BaSeO4	-5.40	-12.86	-7.46	BaSeO4
BaSiF6	-98.36	-130.57	-32.22	BaSiF6
Bassanite	-0.82	-4.52	-3.71	CaSO4:0.5H2O
Bassetite	-24.33	-42.07	-17.74	Fe(UO2)2(PO4)2
BaU2O7	-8.74	13.22	21.96	BaU2O7
BaUO4	-7.75	10.44	18.19	BaUO4
Beidellite-Ca	-0.84	4.61	5.44	Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H	-2.05	2.44	4.49	H.33Al2.33Si3.67O10(OH)2
Beidellite-K	-1.30	3.86	5.16	K.33Al2.33Si3.67O10(OH)2

Beidellite-Mg	-0.99	4.41	5.41	Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na	-0.64	4.86	5.50	Na.33Al2.33Si3.67O10(OH)2
Berlinite	-8.19	-15.46	-7.27	AlPO4
BF3(g)	-64.77	-67.75	-2.98	BF3
Birnessite	0.00	269.79	269.79	Mn8O14:5H2O
Bischofite	-14.78	-10.39	4.39	MgCl2:6H2O
Bixbyite	-3.33	46.86	50.18	Mn2O3
Bloedite	-6.22	-8.70	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-0.16	7.39	7.55	AlO2H
Boltwoodite	-11.83	3.06	14.89	K(H3O)(UO2)SiO4
Boltwoodite-Na	-9.41	5.18	14.58	Na.7K.3(H3O)(UO2)SiO4:H2O
Borax	-0.00	12.04	12.04	Na2(B4O5(OH)4):8H2O
Boric_acid	-0.50	-0.66	-0.16	B(OH)3
Brucite	-4.31	11.97	16.28	Mg(OH)2
Brushite	-16.26	-9.71	6.55	CaHPO4:2H2O
Burkeite	-12.07	-2.58	9.49	Na6CO3(SO4)2
C	-71.88	-93.73	-21.85	C
C(g)	-189.50	-93.73	95.77	C
Ca	-124.88	-28.05	96.83	Ca
Ca(g)	-150.12	-28.05	122.07	Ca
Ca-Al_Pyroxene	-11.99	23.91	35.90	CaAl2SiO6
Ca2Al2O5:8H2O	-18.53	41.04	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-22.32	3.97	26.29	Ca2Cl2(OH)2:H2O
Ca2V2O7	-0.47	16.71	17.18	Ca2V2O7
Ca3(AsO4)2	-53.49	-35.69	17.80	Ca3(AsO4)2
Ca3Al2O6	-58.79	54.25	113.03	Ca3Al2O6
Ca3V2O8	-8.71	29.86	38.57	Ca3V2O8
Ca4Al2Fe2O10	-61.79	104.73	166.52	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-39.94	67.32	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-36.40	67.28	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-38.14	30.19	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-18.97	27.94	46.91	CaAl2O4
CaAl2O4:10H2O	-10.12	27.88	37.99	CaAl2O4:10H2O
CaAl4O7	-25.87	42.73	68.59	CaAl4O7
Calcite	-0.00	1.82	1.82	CaCO3
Carnallite	-21.51	-17.24	4.27	KMgCl3:6H2O
Carnotite	4.07	4.59	0.51	K2(UO2)2(VO4)2
CaSeO3:2H2O	-14.93	-48.58	-33.65	CaSeO3:2H2O
CaSeO4	-4.28	-7.37	-3.09	CaSeO4
CaSO4:0.5H2O(beta)	-0.99	-4.52	-3.54	CaSO4:0.5H2O
CaUO4	0.00	15.94	15.94	CaUO4
CaV2O6	-1.98	3.55	5.53	CaV2O6
Celadonite	0.25	7.56	7.31	KMgAlSi4O10(OH)2
CH4(g)	-145.41	-176.15	-30.74	CH4
Chalcedony	-0.27	-4.03	-3.76	SiO2
Chamosite-7A	-25.88	6.88	32.76	Fe2Al2SiO5(OH)4
Chloromagnesite	-32.16	-10.35	21.82	MgCl2
Chrysotile	-3.17	27.86	31.03	Mg3Si2O5(OH)4
Cl2(g)	-27.12	18.88	45.99	Cl2

```
     Claudetite      -112.83 -157.55  -44.73  As2O3
     Clinochlore-14A  -4.49   62.56   67.05  Mg5Al2Si3O10(OH)8
     Clinochlore-7A   -7.86   62.56   70.42  Mg5Al2Si3O10(OH)8
     Clinoptilolite-Ca  -2.69   -9.98   -7.29
Ca1.7335Al3.45Fe.017Si14.533O36:10.922H2O
     Clinoptilolite-dehy-Ca -38.27   -9.91   28.36
Ca1.7335Al3.45Fe.017Si14.533O36
     Clinoptilolite-dehy-K -42.19  -17.77   24.43
K3.467Al3.45Fe.017Si14.533O36
     Clinoptilolite-dehy-Na -35.47   -7.24   28.23
Na3.467Al3.45Fe.017Si14.533O36
     Clinoptilolite-dehy-NH4-254.96 -642.68 -387.72
(NH4)3.467Al3.45Fe.017Si14.533O36
     Clinoptilolite-hy-Ca  -2.69   -9.99   -7.29
Ca1.7335Al3.45Fe.017Si14.533O36:11.645H2O
     Clinoptilolite-hy-K  -6.58  -17.81  -11.23
K3.467Al3.45Fe.017Si14.533O36:7.499H2O
     Clinoptilolite-hy-Na   0.12   -7.31   -7.43
Na3.467Al3.45Fe.017Si14.533O36:10.877H2O
     Clinoptilolite-K  -6.61  -17.84  -11.23
K3.467Al3.45Fe.017Si14.533O36:10.922H2O
     Clinoptilolite-Na   0.12   -7.31   -7.42
Na3.467Al3.45Fe.017Si14.533O36:10.922H2O
     Clinoptilolite-NH4-219.39 -642.75 -423.36
(NH4)3.467Al3.45Fe.017Si14.533O36:10.922H2O
     Clinozoisite      -6.70   36.40   43.10  Ca2Al3Si3O12(OH)
     CO(g)            -48.21  -52.53   -4.32  CO
     CO2(g)            -3.50  -11.33   -7.83  CO2
     Coesite           -0.81   -4.03   -3.22  SiO2
     Coffinite        -25.33  -42.45  -17.12  USiO4
     Colemanite         0.87   22.39   21.51  Ca2B6O11:5H2O
     Cordierite_anhyd -18.68   33.39   52.07  Mg2Al4Si5O18
     Cordierite_hydr -16.20   33.38   49.59  Mg2Al4Si5O18:H2O
     Corundum          -3.50   14.79   18.29  Al2O3
     Cristobalite(alpha)  -0.55   -4.03   -3.48  SiO2
     Cristobalite(beta)  -0.99   -4.03   -3.03  SiO2
     Cronstedtite-7A -12.79   29.43   42.21  Fe2Fe2SiO5(OH)4
     Daphnite-14A    -59.09   -6.99   52.10  Fe5AlAlSi3O10(OH)8
     Daphnite-7A     -62.47   -6.99   55.48  Fe5AlAlSi3O10(OH)8
     Dawsonite         -0.93    3.41    4.34  NaAlCO3(OH)2
     Diaspore           0.24    7.39    7.15  AlHO2
     Dicalcium_silicate -14.85   22.28   37.13  Ca2SiO4
     Diopside          -3.81   17.07   20.89  CaMgSi2O6
     Dolomite          -0.00    2.47    2.47  CaMg(CO3)2
     Dolomite-dis      -1.54    2.47    4.01  CaMg(CO3)2
     Dolomite-ord       0.01    2.47    2.46  CaMg(CO3)2
     Downeyite        -25.92  -61.72  -35.81  SeO2
     Enstatite         -3.34    7.95   11.29  MgSiO3
     Epidote            1.88   47.67   45.79  Ca2FeAl2Si3O12OH
     Epidote-ord        1.89   47.67   45.78  FeCa2Al2(OH)(SiO4)3
     Epsomite          -3.78   -5.74   -1.96  MgSO4:7H2O
```

Ettringite	-21.98	40.49	62.46	Ca6Al2(SO4)3(OH)12:26H2O
F2(g)	-102.24	-3.53	98.71	F2
Fayalite	-26.96	-7.90	19.06	Fe2SiO4
Fe	-59.15	-43.13	16.02	Fe
Fe(OH)2	-15.83	-1.94	13.89	Fe(OH)2
Fe(OH)3	0.00	18.66	18.66	Fe(OH)3
Fe2(SO4)3	-44.77	-15.68	29.08	Fe2(SO4)3
FeF2	-44.24	-46.67	-2.42	FeF2
FeF3	-42.20	-48.44	-6.24	FeF3
FeO	-15.46	-1.93	13.52	FeO
Ferrite-Ca	2.96	50.49	47.53	CaFe2O4
Ferrite-Dicalcium	-19.19	63.64	82.84	Ca2Fe2O5
Ferrite-Mg	2.25	49.31	47.06	MgFe2O4
Ferrite-Zn	10.80	48.53	37.74	ZnFe2O4
Ferroselite	-152.57	-331.38	-178.81	FeSe2
Ferrosilite	-13.37	-5.96	7.41	FeSiO3
FeSO4	-22.21	-19.61	2.61	FeSO4
FeV2O4	-329.07	-93.94	235.14	FeV2O4
Fluorapatite	-0.00	-25.16	-25.16	Ca5(PO4)3F
Fluorite	-21.51	-31.58	-10.07	CaF2
Forsterite	-7.88	19.93	27.81	Mg2SiO4
Foshagite	-25.28	40.52	65.80	Ca4Si3O9(OH)2:0.5H2O
Frankdicksonite	-31.32	-37.08	-5.76	BaF2
Gaylussite	-6.00	5.16	11.16	CaNa2(CO3)2:5H2O
Gehlenite	-19.16	37.06	56.22	Ca2Al2SiO7
Gibbsite	-0.36	7.38	7.74	Al(OH)3
Gismondine	-2.01	39.71	41.72	Ca2Al4Si4O16:9H2O
Glauberite	-2.03	-7.49	-5.47	Na2Ca(SO4)2
Goethite	5.12	18.66	13.55	FeOOH
Greenalite	-36.45	-13.87	22.58	Fe3Si2O5(OH)4
Grossular	-9.61	42.16	51.78	Ca3Al2(SiO4)3
Gypsum	0.00	-4.53	-4.53	CaSO4:2H2O
Gyrolite	-8.60	14.21	22.80	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-41.21	-41.21	-0.00	H2
H2O(g)	-1.59	-0.01	1.59	H2O
H2S(g)	-140.78	-182.48	-41.70	H2S
Haiweeite	1.56	-5.48	-7.04	Ca(UO2)2(Si2O5)3:5H2O
Halite	-5.38	-3.81	1.56	NaCl
Hatrurite	-37.92	35.43	73.35	Ca3SiO5
Hausmannite	-11.61	49.68	61.29	Mn3O4
HCl(g)	-17.47	-11.17	6.30	HCl
Hedenbergite	-16.36	3.16	19.53	CaFe(SiO3)2
Hematite	11.22	37.33	26.11	Fe2O3
Hercynite	-15.95	12.85	28.80	FeAl2O4
Hexahydrite	-4.01	-5.73	-1.73	MgSO4:6H2O
HI(g)	-35.87	-137.80	-101.93	HI
Hillebrandite	-14.50	22.27	36.77	Ca2SiO3(OH)2:0.17H2O
Hopeite	-1.47	-12.13	-10.66	Zn3(PO4)2:4H2O
HTcO4	-21.37	-15.42	5.95	HTcO4
Huntite	-6.45	3.77	10.22	CaMg3(CO3)4
Hydroboracite	0.84	21.20	20.36	MgCaB6O11:6H2O

Hydromagnesite	-16.20	14.54	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.92	-9.17	11.75	CaCl2
Hydroxylapatite	0.43	-2.79	-3.22	Ca5(OH)(PO4)3
Hydrozincite	3.01	33.32	30.31	Zn5(OH)6(CO3)2
I2	-29.91	-234.40	-204.49	I2
I2(g)	-33.32	-234.40	-201.08	I2
Ice	-0.15	-0.01	0.14	H2O
Illite	-0.40	8.48	8.88	
K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2				
Jadeite	-1.62	6.69	8.31	NaAl(SiO3)2
Jarosite	-4.70	24.95	29.64	KFe3(SO4)2(OH)6
Jarosite-Na	-5.62	27.99	33.61	NaFe3(SO4)2(OH)6
K	-65.77	-16.29	49.48	K
K(g)	-76.37	-16.29	60.08	K
K-Feldspar	-0.00	-0.38	-0.38	KAlSi3O8
K2CO3:1.5H2O	-16.09	-2.72	13.38	K2CO3:1.5H2O
K2O	-75.41	8.62	84.04	K2O
K2Se	-121.74	-176.70	-54.97	K2Se
K2UO4	-22.47	11.40	33.87	K2UO4
K3H(SO4)2	-18.79	-22.41	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-61.22	-33.51	27.71	K8H4(CO3)6:3H2O
Kainite	-12.25	-12.57	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-26.91	-23.64	3.27	KAl(SO4)2
Kalicinite	-7.30	-7.02	0.28	KHCO3
Kalsilite	-3.17	7.68	10.85	KAlSiO4
Kaolinite	0.00	6.72	6.72	Al2Si2O5(OH)4
Karelianite	-56.53	-92.00	-35.47	V2O3
Katoite	-24.74	54.21	78.94	Ca3Al2H12O12
Kieserite	-5.43	-5.70	-0.27	MgSO4:H2O
KMgCl3	-38.45	-17.20	21.25	KMgCl3
KMgCl3:2H2O	-31.17	-17.21	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-9.97	0.29	10.26	KNaCO3:6H2O
KTcO4	-8.83	-11.10	-2.27	KTcO4
KUO2AsO4	-26.31	-30.48	-4.17	KUO2AsO4
Kyanite	-4.85	10.76	15.61	Al2SiO5
Lansfordite	-4.22	0.62	4.84	MgCO3:5H2O
Larnite	-16.14	22.28	38.42	Ca2SiO4
Laumontite	-1.71	11.80	13.51	CaAl2Si4O12:4H2O
Lawrencite	-33.31	-24.26	9.05	FeCl2
Lawsonite	-2.23	19.87	22.11	CaAl2Si2O7(OH)2:H2O
Leonite	-10.66	-14.77	-4.11	K2Mg(SO4)2:4H2O
Lime	-19.42	13.15	32.57	CaO
Magnesite	-1.62	0.65	2.27	MgCO3
Magnetite	-1.05	35.40	36.45	Fe3O4
Manganite	-1.98	23.42	25.41	MnO(OH)
Manganosite	-15.09	2.83	17.92	MnO
Margarite	-6.26	34.66	40.93	CaAl4Si2O10(OH)2
Maximum_Microcline	0.00	-0.38	-0.38	KAlSi3O8
Mayenite	-232.81	261.34	494.15	Ca12Al14O33
Melanterite	-17.25	-19.65	-2.40	FeSO4:7H2O
Mercallite	-11.93	-13.36	-1.44	KHSO4
Merwinite	-25.03	43.38	68.41	MgCa3(SiO4)2

```
     Mesolite            2.69   16.18   13.49
Na.676Ca.657Al1.99Si3.01O10:2.647H2O
     Mg               -108.75  -29.22   79.52  Mg
     Mg(g)            -128.47  -29.22   99.25  Mg
     Mg1.25SO4(OH)0.5:0.5H2O  -7.90   -2.71    5.20
Mg1.25SO4(OH)0.5:0.5H2O
     Mg1.5SO4(OH)       -8.92    0.29    9.21  Mg1.5SO4(OH)
     Mg2V2O7           -11.64   14.36   25.99  Mg2V2O7
     MgCl2:2H2O        -23.09  -10.36   12.73  MgCl2:2H2O
     MgCl2:4H2O        -17.68  -10.37    7.30  MgCl2:4H2O
     MgCl2:H2O         -26.43  -10.35   16.07  MgCl2:H2O
     MgOHCl            -15.08    0.81   15.89  MgOHCl
     MgSeO3            -22.40  -49.74  -27.34  MgSeO3
     MgSeO3:6H2O       -17.33  -49.78  -32.45  MgSeO3:6H2O
     MgSO4             -10.52   -5.69    4.83  MgSO4
     MgUO4              -8.23   14.76   22.99  MgUO4
     MgV2O6             -8.67    2.38   11.05  MgV2O6
     Minnesotaite      -35.75  -21.92   13.83  Fe3Si4O10(OH)2
     Mirabilite         -1.88   -3.04   -1.15  Na2SO4:10H2O
     Misenite          -78.16  -89.23  -11.08  K8H6(SO4)7
     Mn                -78.31  -38.37   39.94  Mn
     Mn(OH)2(am)       -12.49    2.82   15.31  Mn(OH)2
     Mn(OH)3            -8.50   23.42   31.92  Mn(OH)3
     Mn3(PO4)2         -38.04  -37.22    0.82  Mn3(PO4)2
     MnCl2:2H2O        -23.51  -19.51    4.00  MnCl2:2H2O
     MnCl2:4H2O        -22.28  -19.52    2.75  MnCl2:4H2O
     MnCl2:H2O         -25.05  -19.50    5.54  MnCl2:H2O
     MnHPO4             -7.08  -20.03  -12.95  MnHPO4
     MnO2(gamma)         0.93   44.03   43.10  MnO2
     MnSe             -105.55 -182.50  -76.95  MnSe
     MnSeO3            -22.61  -58.89  -36.29  MnSeO3
     MnSeO3:2H2O       -23.56  -58.91  -35.35  MnSeO3:2H2O
     MnSO4             -17.45  -14.84    2.61  MnSO4
     MnV2O6            -11.59   -6.77    4.82  MnV2O6
     Molysite          -41.31  -14.82   26.49  FeCl3
     Monohydrocalcite   -0.86    1.82    2.68  CaCO3:H2O
     Monticellite       -8.43   21.10   29.53  CaMgSiO4
     Montmor-Ca          0.01    2.35    2.34
Ca.165Mg.33Al1.67Si4O10(OH)2
     Montmor-K          -0.39    1.60    1.99
K.33Mg.33Al1.67Si4O10(OH)2
     Montmor-Mg         -0.08    2.16    2.23
Mg.495Al1.67Si4O10(OH)2
     Montmor-Na          0.28    2.61    2.33
Na.33Mg.33Al1.67Si4O10(OH)2
     Mordenite          -1.63   -6.99   -5.36
Ca.2895Na.361Al.94Si5.06O12:3.468H2O
     Mordenite-dehy    -16.74   -6.97    9.77
Ca.2895Na.361Al.94Si5.06O12
     Muscovite           0.95   14.40   13.45  KAl3Si3O10(OH)2
     N2(g)             -17.75 -228.24 -210.49  N2
     Na                -59.12  -13.25   45.87  Na
```

Na(g)	-72.61	-13.25	59.36	Na
Na2CO3	-7.80	3.37	11.16	Na2CO3
Na2CO3:7H2O	-6.62	3.32	9.94	Na2CO3:7H2O
Na2O	-52.72	14.70	67.42	Na2O
Na2Se	-116.21	-170.63	-54.42	Na2Se
Na2Se2	-163.89	-314.75	-150.86	Na2Se2
Na2SiO3	-11.53	10.67	22.20	Na2SiO3
Na2U2O7	-2.33	20.26	22.59	Na2U2O7
Na2UO4(alpha)	-12.54	17.48	30.02	Na2UO4
Na3H(SO4)2	-12.41	-13.30	-0.89	Na3H(SO4)2
Na3UO4	-50.53	4.23	54.76	Na3UO4
Na4Ca(SO4)3:2H2O	-4.59	-10.48	-5.89	Na4Ca(SO4)3:2H2O
Na4SiO4	-45.23	25.36	70.60	Na4SiO4
Na4UO2(CO3)3	-5.85	-1.81	4.04	Na4UO2(CO3)3
Na6Si2O7	-65.50	36.03	101.53	Na6Si2O7
NaFeO2	-6.89	26.02	32.90	NaFeO2
Nahcolite	-3.84	-3.98	-0.14	NaHCO3
NaTcO4	-9.59	-8.07	1.52	NaTcO4
Natrolite	-1.00	17.39	18.39	Na2Al2Si3O10:2H2O
Natron	-6.28	3.30	9.59	Na2CO3:10H2O
Natrosilite	-11.42	6.64	18.07	Na2Si2O5
NaUO3	-17.32	-10.47	6.85	NaUO3
Nepheline	-3.04	10.71	13.75	NaAlSiO4
Nesquehonite	-4.66	0.63	5.29	MgCO3:3H2O
NH3(g)	-67.81	-175.93	-108.13	NH3
NH4HSe	-163.03	-361.26	-198.23	NH4HSe
Ningyoite	-32.12	-70.98	-38.86	CaUP2O8:2H2O
Niter	-6.58	-6.81	-0.22	KNO3
Nitrobarite	-12.08	-14.57	-2.49	Ba(NO3)2
NO(g)	-24.39	-72.92	-48.53	NO
NO2(g)	-18.57	-31.72	-13.15	NO2
Nontronite-Ca	12.85	27.16	14.31	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	11.64	24.98	13.35	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	12.38	26.41	14.02	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	12.69	26.96	14.27	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	13.05	27.41	14.36	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-0.70	82.40	83.10	O2
Okenite	-5.23	5.09	10.31	CaSi2O4(OH)2:H2O
Orpiment	-499.45	-704.98	-205.54	As2S3
Oxychloride-Mg	-13.07	12.76	25.83	Mg2Cl(OH)3:4H2O
P	-150.41	-125.85	24.56	P
Paragonite	0.06	17.44	17.38	NaAl3Si3O10(OH)2
Pargasite	-22.13	79.57	101.70	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrite	-4.34	-5.73	-1.39	MgSO4:5H2O
Periclase	-9.35	11.98	21.33	MgO
Phlogopite	-1.75	35.55	37.30	KAlMg3Si3O10(OH)2
Picromerite	-10.34	-14.78	-4.44	K2Mg(SO4)2:6H2O

Pirssonite	-6.14	5.18	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-9.48	-23.79	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-9.40	13.15	22.55	Ca(OH)2
Prehnite	-3.79	29.00	32.79	Ca2Al2Si3O10(OH)2
Pseudowollastonite	-4.84	9.13	13.96	CaSiO3
Pu	-174.14	-108.33	65.81	Pu
Pu(HPO4)2	-25.31	-71.64	-46.33	Pu(HPO4)2
Pu(OH)3	-33.43	-46.54	-13.11	Pu(OH)3
Pu(OH)4	-8.14	-25.94	-17.81	Pu(OH)4
Pu2O3	-70.07	-93.06	-22.98	Pu2O3
PuF3	-67.83	-113.63	-45.80	PuF3
PuF4	-83.55	-115.40	-31.85	PuF4
PuO2	0.00	-25.93	-25.93	PuO2
PuO2(OH)2	-4.59	15.27	19.86	PuO2(OH)2
PuO2HPO4	-11.24	-7.58	3.66	PuO2HPO4
PuO2OH(am)	-10.79	-5.33	5.46	PuO2OH
Pyrite	-242.00	-325.69	-83.69	FeS2
Pyrolusite	2.47	44.03	41.56	MnO2
Pyrophyllite	-1.62	-1.33	0.29	Al2Si4O10(OH)2
Pyrrhotite	-146.96	-184.41	-37.45	FeS
Quartz	0.00	-4.03	-4.03	SiO2
Rankinite	-20.42	31.40	51.82	Ca3Si2O7
Realgar	-200.74	-281.85	-81.11	AsS
Rhodochrosite	-8.28	-8.50	-0.22	MnCO3
Rhodonite	-10.89	-1.20	9.69	MnSiO3
Ripidolite-14A	-26.04	34.74	60.78	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	-29.42	34.74	64.16	Mg3Fe2Al2Si3O10(OH)8
Rutherfordine	-4.43	-8.55	-4.12	UO2CO3
S	-105.46	-141.28	-35.82	S
S2(g)	-224.80	-282.55	-57.75	S2
Saleeite	-8.69	-28.16	-19.48	Mg(UO2)2(PO4)2
Sanbornite	-9.80	-0.40	9.41	BaSi2O5
Sanidine_high	-1.20	-0.38	0.82	KAlSi3O8
Saponite-Ca	-0.39	25.75	26.14	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	-1.60	23.58	25.18	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	-0.85	25.01	25.86	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	-0.54	25.56	26.10	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	-0.19	26.01	26.20	Na.33Mg3Al.33Si3.67O10(OH)2
Scacchite	-28.24	-19.50	8.74	MnCl2
Schoepite	-2.07	2.77	4.83	UO3:2H2O
Schoepite-dehy(.393)	-3.95	2.78	6.72	UO3:.393H2O
Schoepite-dehy(.648)	-3.43	2.78	6.21	UO3:.648H2O
Schoepite-dehy(.85)	-2.32	2.78	5.10	UO3:.85H2O
Schoepite-dehy(.9)	-2.24	2.78	5.02	UO3:.9H2O
Schoepite-dehy(1.0)	-2.33	2.78	5.10	UO3:H2O
Scolecite	0.09	15.84	15.75	CaAl2Si3O10:3H2O
Se	-55.21	-144.12	-88.92	Se

Se2O5	-62.72	-82.24	-19.53	Se2O5
SeCl4	-91.69	-106.37	-14.68	SeCl4
Sellaite	-23.31	-32.76	-9.44	MgF2
SeO3	-39.68	-20.52	19.16	SeO3
Sepiolite	-6.52	23.70	30.22	Mg4Si6O15(OH)2:6H2O
Shcherbinaite	-8.15	-9.60	-1.45	V2O5
Si	-149.30	-86.43	62.87	Si
Si(g)	-220.37	-86.43	133.94	Si
Siderite	-13.04	-13.26	-0.22	FeCO3
SiF4(g)	-78.26	-93.50	-15.24	SiF4
Sillimanite	-5.49	10.76	16.24	Al2SiO5
SiO2(am)	-1.29	-4.03	-2.74	SiO2
Sklodowskite	-4.35	9.44	13.79	
Mg(H3O)2(UO2)2(SiO4)2:4H2O				
Smectite-high-Fe-Mg	-6.27	13.60	19.88	
Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12				
Smectite-low-Fe-Mg	-3.41	9.56	12.98	
Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12				
Smithsonite	-0.57	-0.13	0.44	ZnCO3
SO2(g)	-53.56	-58.87	-5.32	SO2
Soddyite	1.13	1.52	0.39	(UO2)2SiO4:2H2O
Sphalerite	-126.10	-171.28	-45.18	ZnS
Spinel	-10.84	26.76	37.61	Al2MgO4
Starkeyite	-4.72	-5.72	-1.00	MgSO4:4H2O
Stilbite	2.22	3.03	0.81	
Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O				
Stilleite	-83.89	-174.13	-90.24	ZnSe
Strengite	-5.82	-4.20	1.63	FePO4:2H2O
Sylvite	-7.68	-6.85	0.83	KCl
Syngenite	-5.97	-13.57	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-47.09	-29.94	17.14	Mg2CaCl6:12H2O
Talc	-1.17	19.81	20.99	Mg3Si4O10(OH)2
Tb	-158.69	-41.80	116.89	Tb
Tb(OH)3	4.31	19.99	15.69	Tb(OH)3
Tb(OH)3(am)	1.21	19.99	18.79	Tb(OH)3
Tb2(CO3)3	9.24	6.02	-3.21	Tb2(CO3)3
Tb2O3	-7.09	40.01	47.10	Tb2O3
TbF3:.5H2O	-30.40	-47.10	-16.70	TbF3:.5H2O
TbPO4:10H2O	9.07	-2.91	-11.98	TbPO4:10H2O
Tc	-102.70	-159.62	-56.92	Tc
Tc(OH)2	-63.82	-118.42	-54.61	Tc(OH)2
Tc(OH)3	-50.20	-97.83	-47.62	Tc(OH)3
Tc2O7	-43.93	-30.83	13.10	Tc2O7
Tc2O7(g)	-52.18	-30.83	21.35	Tc2O7
Tc2S7	-841.94	-1308.17	-466.23	Tc2S7
Tc3O4	-158.18	-314.05	-155.87	Tc3O4
Tc4O7	-181.31	-350.07	-168.76	Tc4O7
TcO2:2H2O(am)	-40.01	-77.23	-37.22	TcO2:2H2O
TcO3	-23.19	-36.01	-12.83	TcO3
TcOH	-82.54	-139.02	-56.48	TcOH
TcS2	-275.79	-442.17	-166.38	TcS2
TcS3	-373.14	-583.45	-210.30	TcS3

Tephroite	-21.40	1.63	23.02	Mn2SiO4
Thenardite	-2.62	-2.98	-0.36	Na2SO4
Thermonatrite	-7.58	3.36	10.94	Na2CO3:H2O
Tobermorite-11A	-23.82	41.57	65.39	Ca5Si6H11O22.5
Tobermorite-14A	-22.08	41.53	63.61	Ca5Si6H21O27.5
Tobermorite-9A	-27.27	41.58	68.86	Ca5Si6H6O20
Todorokite	-0.29	225.78	226.07	Mn7O12:3H2O
Tremolite	-6.96	53.96	60.93	Ca2Mg5Si8O22(OH)2
Tridymite	-0.19	-4.03	-3.84	SiO2
Troilite	-146.86	-184.41	-37.55	FeS
Trona-K	-18.29	-6.70	11.59	K2NaH(CO3)2:2H2O
Tyuyamunite	5.60	9.12	3.52	Ca(UO2)2(VO4)2
U	-204.60	-120.82	83.77	U
U(CO3)2	-59.55	-61.08	-1.53	U(CO3)2
U(g)	-290.15	-120.82	169.33	U
U(HPO4)2:4H2O	-42.18	-84.15	-41.98	U(HPO4)2:4H2O
U(OH)2SO4	-43.97	-56.10	-12.12	U(OH)2SO4
U(SO3)2	-117.59	-156.17	-38.58	U(SO3)2
U(SO4)2	-53.18	-73.76	-20.58	U(SO4)2
U(SO4)2:4H2O	-53.19	-73.79	-20.60	U(SO4)2:4H2O
U(SO4)2:8H2O	-52.20	-73.81	-21.62	U(SO4)2:8H2O
U2C3	-591.67	-522.84	68.84	U2C3
U2Cl10(g)	-226.90	-147.27	79.64	U2Cl10
U2Cl8(g)	-230.32	-166.14	64.17	U2Cl8
U2F10(g)	-243.88	-259.31	-15.44	U2F10
U2F9	-201.36	-257.55	-56.19	U2F9
U2O2Cl5	-120.71	-112.05	8.66	U2O2Cl5
U2O3F6	-126.11	-128.64	-2.53	U2O3F6
U2S3	-571.43	-665.47	-94.04	U2S3
U2Se3	-448.59	-674.02	-225.43	U2Se3
U3As4	-911.92	-924.78	-12.86	U3As4
U3O5F8	-167.72	-170.60	-2.88	U3O5F8
U3P4	-1070.70	-865.89	204.81	U3P4
U3S5	-891.49	-1068.85	-177.36	U3S5
U3Se4	-661.55	-938.96	-277.41	U3Se4
U3Se5	-691.94	-1083.09	-391.15	U3Se5
U4F17	-379.61	-513.33	-133.72	U4F17
U5O12Cl	-74.06	-100.26	-26.20	U5O12Cl
UAs	-269.22	-261.40	7.82	UAs
UAs2	-372.91	-401.98	-29.06	UAs2
UC	-259.15	-214.55	44.60	UC
UC1.94(alpha)	-328.75	-302.66	26.09	UC1.94
UCl(g)	-245.66	-111.38	134.28	UCl
UCl2(g)	-199.70	-101.95	97.75	UCl2
UCl2F2	-92.84	-105.48	-12.64	UCl2F2
UCl2I2	-134.93	-336.34	-201.41	UCl2I2
UCl3	-105.78	-92.51	13.27	UCl3
UCl3(g)	-151.39	-92.51	58.88	UCl3
UCl3F	-95.47	-94.28	1.19	UCl3F
UCl3I	-114.86	-209.71	-94.84	UCl3I
UCl4	-95.94	-83.07	12.87	UCl4
UCl4(g)	-120.37	-83.07	37.30	UCl4

UCl5	-109.38	-73.63	35.75	UCl5
UCl5(g)	-126.60	-73.63	52.97	UCl5
UCl6	-121.69	-64.20	57.50	UCl6
UCl6(g)	-127.56	-64.20	63.37	UCl6
UClF3	-90.05	-116.69	-26.64	UClF3
UClI3	-155.18	-462.98	-307.80	UClI3
UF(g)	-241.34	-122.59	118.76	UF
UF2(g)	-210.68	-124.36	86.32	UF2
UF3	-106.96	-126.12	-19.17	UF3
UF3(g)	-173.61	-126.12	47.49	UF3
UF4	-89.58	-127.89	-38.31	UF4
UF4(g)	-133.37	-127.89	5.48	UF4
UF4:2.5H2O	-85.41	-127.91	-42.49	UF4:2.5H2O
UF5(alpha)	-115.23	-129.66	-14.42	UF5
UF5(beta)	-114.91	-129.66	-14.75	UF5
UF5(g)	-134.46	-129.66	4.80	UF5
UF6	-148.73	-131.42	17.31	UF6
UF6(g)	-149.57	-131.42	18.15	UF6
UH3(beta)	-253.71	-182.63	71.07	UH3
UI(g)	-270.00	-238.02	31.98	UI
UI2(g)	-241.06	-355.22	-114.15	UI2
UI3	-167.71	-472.41	-304.71	UI3
UI3(g)	-214.31	-472.41	-258.11	UI3
UI4	-174.52	-589.61	-415.09	UI4
UI4(g)	-199.53	-589.61	-390.09	UI4
UN	-167.02	-234.94	-67.93	UN
UN1.59(alpha)	-159.46	-302.27	-142.81	UN1.59
UN1.73(alpha)	-157.98	-318.25	-160.27	UN1.73
UO(g)	-205.27	-79.62	125.65	UO
UO2(am)	-29.48	-38.42	-8.94	UO2
UO2(AsO3)2	-79.28	-72.37	6.91	UO2(AsO3)2
UO2(g)	-121.02	-38.42	82.60	UO2
UO2(IO3)2	-18.31	-25.61	-7.29	UO2(IO3)2
UO2(NO3)2	-31.40	-19.45	11.95	UO2(NO3)2
UO2(NO3)2:2H2O	-24.37	-19.46	4.91	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-23.15	-19.47	3.68	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-21.78	-19.49	2.29	UO2(NO3)2:6H2O
UO2(NO3)2:H2O	-27.96	-19.46	8.50	UO2(NO3)2:H2O
UO2(OH)2(beta)	-2.17	2.78	4.95	UO2(OH)2
UO2(PO3)2	-26.58	-42.92	-16.34	UO2(PO3)2
UO2.25	-18.02	-28.12	-10.10	UO2.25
UO2.25(beta)	-18.09	-28.12	-10.02	UO2.25
UO2.3333(beta)	-32.22	-49.37	-17.15	(UO2.3333)2
UO2.6667	-17.53	-21.90	-4.37	(UO2.6667)2
UO2Cl	-26.97	-28.98	-2.02	UO2Cl
UO2Cl2	-31.65	-19.54	12.11	UO2Cl2
UO2Cl2(g)	-67.48	-19.54	47.93	UO2Cl2
UO2Cl2:3H2O	-25.17	-19.56	5.61	UO2Cl2:3H2O
UO2Cl2:H2O	-27.83	-19.55	8.28	UO2Cl2:H2O
UO2ClOH:2H2O	-10.70	-8.40	2.30	UO2ClOH:2H2O
UO2CO3	-4.42	-8.55	-4.13	UO2CO3
UO2F2	-34.69	-41.95	-7.27	UO2F2

UO2F2(g)	-76.58	-41.95	34.63	UO2F2
UO2F2:3H2O	-34.59	-41.97	-7.38	UO2F2:3H2O
UO2FOH	-17.74	-19.59	-1.85	UO2FOH
UO2FOH:2H2O	-16.93	-19.60	-2.67	UO2FOH:2H2O
UO2FOH:H2O	-17.31	-19.60	-2.29	UO2FOH:H2O
UO2HPO4	-7.39	-20.07	-12.68	UO2HPO4
UO2HPO4:4H2O	-7.07	-20.10	-13.03	UO2HPO4:4H2O
UO2SO3	-43.72	-56.09	-12.37	UO2SO3
UO2SO4	-16.82	-14.89	1.93	UO2SO4
UO2SO4:2.5H2O	-13.40	-14.91	-1.50	UO2SO4:2.5H2O
UO2SO4:3.5H2O	-13.42	-14.91	-1.49	UO2SO4:3.5H2O
UO2SO4:3H2O	-13.50	-14.91	-1.41	UO2SO4:3H2O
UO2SO4:H2O	-8.83	-14.90	-6.07	UO2SO4:H2O
UO3(alpha)	-5.86	2.78	8.64	UO3
UO3(beta)	-5.53	2.78	8.31	UO3
UO3(g)	-68.17	2.78	70.95	UO3
UO3(gamma)	-4.93	2.78	7.71	UO3
UO3:.9H2O(alpha)	-2.24	2.78	5.02	UO3:.9H2O
UO3:2H2O	-2.07	2.77	4.84	UO3:2H2O
UOCl	-80.85	-70.18	10.67	UOCl
UOCl2	-57.12	-60.75	-3.63	UOCl2
UOCl3	-62.41	-51.31	11.10	UOCl3
UOF2	-55.95	-83.15	-27.20	UOF2
UOF2:H2O	-55.40	-83.16	-27.76	UOF2:H2O
UOF4	-91.25	-86.69	4.56	UOF4
UOF4(g)	-110.90	-86.69	24.21	UOF4
UOFOH	-42.81	-60.79	-17.98	UOFOH
UOFOH:.5H2O	-42.36	-60.79	-18.43	UOFOH:.5H2O
UP	-308.44	-246.68	61.76	UP
UP2	-453.82	-372.53	81.29	UP2
UP2O7	-42.00	-84.12	-42.12	UP2O7
UP2O7:20H2O	-46.57	-84.25	-37.68	UP2O7:20H2O
UPO5	-19.58	-40.67	-21.09	UPO5
Uraninite	-24.54	-38.42	-13.88	UO2
Uranium-selenide	-211.29	-264.95	-53.65	USe
Uranocircite	-12.66	-32.48	-19.82	Ba(UO2)2(PO4)2
Uranophane	-6.63	10.65	17.29	Ca(UO2)2(SiO3)2(OH)2
US	-253.83	-262.10	-8.27	US
US1.9	-315.71	-389.25	-73.53	US1.9
US2	-324.55	-403.37	-78.83	US2
US3	-426.84	-544.65	-117.81	US3
USe2(alpha)	-240.19	-409.07	-168.88	USe2
USe2(beta)	-240.04	-409.07	-169.03	USe2
USe3	-291.14	-553.20	-262.05	USe3
V	-127.54	-107.80	19.74	V
V2O4	-25.53	-50.80	-25.27	V2O4
V3O5	-68.49	-117.40	-48.91	V3O5
V4O7	-82.35	-142.80	-60.45	V4O7
Vivianite	-46.83	-51.55	-4.72	Fe3(PO4)2:8H2O
Wairakite	-6.10	11.82	17.92	CaAl2Si4O10(OH)4
Weeksite	-25.38	-10.01	15.38	K2(UO2)2(Si2O5)3:4H2O
Whitlockite	-1.92	-6.24	-4.32	Ca3(PO4)2

Witherite	-0.65	-3.67	-3.02	BaCO3
Wollastonite	-4.60	9.13	13.72	CaSiO3
Wurtzite	-128.40	-171.28	-42.88	ZnS
Wustite	-13.43	0.35	13.78	Fe.947O
Xonotlite	-36.99	54.75	91.74	Ca6Si6O17(OH)2
Yb	-154.73	-42.60	112.13	Yb
Yb(OH)3	4.51	19.19	14.69	Yb(OH)3
Yb(OH)3(am)	0.21	19.19	18.99	Yb(OH)3
Yb2(CO3)3	6.73	4.42	-2.31	Yb2(CO3)3
Yb2O3	-9.39	38.41	47.80	Yb2O3
YbF3:.5H2O	-31.90	-47.90	-16.00	YbF3:.5H2O
YbPO4:10H2O	8.07	-3.71	-11.78	YbPO4:10H2O
Zincite	0.00	11.20	11.20	ZnO
Zn	-55.79	-30.00	25.79	Zn
Zn(BO2)2	1.59	9.90	8.31	Zn(BO2)2
Zn(ClO4)2:6H2O	-62.62	318.45	381.06	Zn(ClO4)2:6H2O
Zn(g)	-72.41	-30.00	42.41	Zn
Zn(IO3)2	-11.87	-17.19	-5.32	Zn(IO3)2
Zn(NO3)2:6H2O	-14.47	-11.07	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-0.74	11.19	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-0.47	11.19	11.66	Zn(OH)2
Zn(OH)2(gamma)	-0.69	11.19	11.88	Zn(OH)2
Zn2(OH)3Cl	-4.07	11.23	15.29	Zn2(OH)3Cl
Zn2SiO4	4.53	18.37	13.84	Zn2SiO4
Zn2SO4(OH)2	-2.86	4.72	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-50.86	-41.55	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-20.84	-1.75	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-8.93	33.74	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.20	-11.13	7.08	ZnCl2
ZnCl2(NH3)2	-136.14	-362.99	-226.85	ZnCl2(NH3)2
ZnCl2(NH3)4	-268.45	-714.85	-446.40	ZnCl2(NH3)4
ZnCl2(NH3)6	-402.44	-1066.71	-664.28	ZnCl2(NH3)6
ZnCO3:H2O	-0.28	-0.14	0.14	ZnCO3:H2O
ZnF2	-33.04	-33.54	-0.49	ZnF2
ZnI2	-49.13	-264.40	-215.27	ZnI2
ZnSeO3:H2O	-14.76	-50.53	-35.77	ZnSeO3:H2O
ZnSO4	-10.01	-6.47	3.53	ZnSO4
ZnSO4:6H2O	-4.81	-6.51	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.64	-6.52	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-5.93	-6.48	-0.55	ZnSO4:H2O
Zoisite	-6.74	36.40	43.14	Ca2Al3(SiO4)3OH

End of simulation.

Reading input data for simulation 3.

End of run.