
Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat
SOLUTION 1 Flujo 1
temp 25
pH 3.098
pe 17
redox pe
units mg/l
density 1
Cl 46.4
S(6) 830
Al 11.6
As 1.7
Ca 78.4
Cu 21.3
Fe 133.5
K 30.3
Mg 8.6
Mn 14.1
Na 19.5
Zn 5.2
C(4) 0
water 1 # kg
SOLUTION 2 Inter 3
temp 25
units mg/l
pe 12
pH 2.29
Cl 39.1
S(6) 1113.00
Al 34.60
As 0.01
Ca 305.00
Cu 0.13
Fe 12.16
K 8.67
Mg 29.67
Mn 13.97
Na 65.26
Zn 0.02
C(4) 0
MIX 1
1 1

```

2      3
SELECTED_OUTPUT
file          DAM_AGUASUP
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 1

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

| Elements | Molality | Moles |
|----------|------------|------------|
| Al | 4.304e-004 | 4.304e-004 |
| As | 2.272e-005 | 2.272e-005 |
| Ca | 1.959e-003 | 1.959e-003 |
| Cl | 1.310e-003 | 1.310e-003 |
| Cu | 3.356e-004 | 3.356e-004 |
| Fe | 2.393e-003 | 2.393e-003 |
| K | 7.759e-004 | 7.759e-004 |
| Mg | 3.543e-004 | 3.543e-004 |
| Mn | 2.570e-004 | 2.570e-004 |
| Na | 8.492e-004 | 8.492e-004 |
| S(6) | 8.652e-003 | 8.652e-003 |
| Zn | 7.962e-005 | 7.962e-005 |

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

```

pH = 3.098
pe = 17.000
Activity of water = 1.000
Ionic strength = 2.715e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -3.600e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -3.759e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -13.38
Iterations = 9
Total H = 1.110544e+002
Total O = 5.556248e+001

```

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|----------------|------------|------------|-----------------|-----------------|--------------|
| H+ | 9.068e-004 | 7.980e-004 | -3.042 | -3.098 | -0.056 |
| OH- | 1.417e-011 | 1.207e-011 | -10.849 | -10.918 | -0.070 |
| H2O | 5.553e+001 | 9.997e-001 | 1.744 | -0.000 | 0.000 |
| Al | 4.304e-004 | | | | |
| AlSO4+ | 2.135e-004 | 1.825e-004 | -3.671 | -3.739 | -0.068 |
| Al+3 | 1.537e-004 | 4.763e-005 | -3.813 | -4.322 | -0.509 |
| Al(SO4)2- | 6.205e-005 | 5.304e-005 | -4.207 | -4.275 | -0.068 |
| AlOH+2 | 1.244e-006 | 6.684e-007 | -5.905 | -6.175 | -0.270 |
| Al(OH)2+ | 2.275e-009 | 1.944e-009 | -8.643 | -8.711 | -0.068 |
| Al2(OH)2+4 | 7.923e-010 | 7.265e-011 | -9.101 | -10.139 | -1.038 |
| HALO2 | 3.546e-012 | 3.546e-012 | -11.450 | -11.450 | 0.000 |
| Al3(OH)4+5 | 1.360e-013 | 3.505e-015 | -12.866 | -14.455 | -1.589 |
| AlO2- | 1.781e-015 | 1.522e-015 | -14.749 | -14.818 | -0.068 |
| NaAlO2 | 2.057e-019 | 2.057e-019 | -18.687 | -18.687 | 0.000 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -52.670 | -55.785 | -3.115 |

| | | | | | | |
|----------|------------|------------|----------|----------|--------|--|
| As(-3) | 0.000e+000 | | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -151.853 | -151.853 | 0.000 | |
| As(3) | 9.018e-027 | | | | | |
| HAsO2 | 4.812e-027 | 4.812e-027 | -26.318 | -26.318 | 0.000 | |
| As(OH)3 | 4.206e-027 | 4.206e-027 | -26.376 | -26.376 | 0.000 | |
| H2AsO3- | 3.771e-033 | 3.223e-033 | -32.424 | -32.492 | -0.068 | |
| AsO2- | 3.606e-033 | 3.082e-033 | -32.443 | -32.511 | -0.068 | |
| AsO2OH-2 | 0.000e+000 | 0.000e+000 | -40.128 | -40.404 | -0.276 | |
| As(5) | 2.272e-005 | | | | | |
| H2AsO4- | 2.027e-005 | 1.733e-005 | -4.693 | -4.761 | -0.068 | |
| H3AsO4 | 2.436e-006 | 2.436e-006 | -5.613 | -5.613 | 0.000 | |
| HAsO4-2 | 6.805e-009 | 3.605e-009 | -8.167 | -8.443 | -0.276 | |
| AsO4-3 | 4.856e-017 | 1.159e-017 | -16.314 | -16.936 | -0.622 | |
| Ca | 1.959e-003 | | | | | |
| Ca+2 | 1.500e-003 | 8.374e-004 | -2.824 | -3.077 | -0.253 | |
| CaSO4 | 4.580e-004 | 4.580e-004 | -3.339 | -3.339 | 0.000 | |
| CaCl+ | 2.306e-007 | 1.971e-007 | -6.637 | -6.705 | -0.068 | |
| CaCl2 | 2.574e-010 | 2.574e-010 | -9.589 | -9.589 | 0.000 | |
| CaOH+ | 1.734e-013 | 1.482e-013 | -12.761 | -12.829 | -0.068 | |
| Cl(-1) | 1.310e-003 | | | | | |
| Cl- | 1.309e-003 | 1.110e-003 | -2.883 | -2.955 | -0.071 | |
| CuCl+ | 4.495e-007 | 3.842e-007 | -6.347 | -6.415 | -0.068 | |
| MnCl+ | 2.615e-007 | 2.235e-007 | -6.583 | -6.651 | -0.068 | |
| CaCl+ | 2.306e-007 | 1.971e-007 | -6.637 | -6.705 | -0.068 | |
| HCl | 1.990e-007 | 1.990e-007 | -6.701 | -6.701 | 0.000 | |
| NaCl | 1.382e-007 | 1.382e-007 | -6.859 | -6.859 | 0.000 | |
| MgCl+ | 1.323e-007 | 1.131e-007 | -6.878 | -6.946 | -0.068 | |
| ZnCl+ | 6.734e-008 | 5.756e-008 | -7.172 | -7.240 | -0.068 | |
| FeCl+2 | 3.035e-008 | 1.630e-008 | -7.518 | -7.788 | -0.270 | |
| KCl | 2.383e-008 | 2.383e-008 | -7.623 | -7.623 | 0.000 | |
| FeCl2+ | 1.715e-008 | 1.466e-008 | -7.766 | -7.834 | -0.068 | |
| CaCl2 | 2.574e-010 | 2.574e-010 | -9.589 | -9.589 | 0.000 | |
| CuCl2 | 2.247e-010 | 2.247e-010 | -9.648 | -9.648 | 0.000 | |
| ZnCl2 | 7.466e-011 | 7.466e-011 | -10.127 | -10.127 | 0.000 | |
| FeCl+ | 8.697e-012 | 7.434e-012 | -11.061 | -11.129 | -0.068 | |
| Zn(OH)Cl | 1.233e-012 | 1.233e-012 | -11.909 | -11.909 | 0.000 | |
| MnCl3- | 7.044e-014 | 6.021e-014 | -13.152 | -13.220 | -0.068 | |
| ZnCl3- | 5.357e-014 | 4.579e-014 | -13.271 | -13.339 | -0.068 | |
| ZnCl4-2 | 7.275e-016 | 3.854e-016 | -15.138 | -15.414 | -0.276 | |
| FeCl2 | 4.430e-017 | 4.430e-017 | -16.354 | -16.354 | 0.000 | |
| FeCl4- | 2.542e-017 | 2.173e-017 | -16.595 | -16.663 | -0.068 | |
| CuCl2- | 6.618e-020 | 5.657e-020 | -19.179 | -19.247 | -0.068 | |
| CuCl4-2 | 9.814e-021 | 5.199e-021 | -20.008 | -20.284 | -0.276 | |
| CuCl3-2 | 7.615e-022 | 4.034e-022 | -21.118 | -21.394 | -0.276 | |
| FeCl4-2 | 2.980e-022 | 1.578e-022 | -21.526 | -21.802 | -0.276 | |
| Cl(1) | 4.019e-017 | | | | | |
| HClO | 4.019e-017 | 4.019e-017 | -16.396 | -16.396 | 0.000 | |
| ClO- | 1.589e-021 | 1.358e-021 | -20.799 | -20.867 | -0.068 | |
| Cl(3) | 4.974e-032 | | | | | |
| HClO2 | 2.497e-032 | 2.497e-032 | -31.603 | -31.603 | 0.000 | |
| ClO2- | 2.476e-032 | 2.117e-032 | -31.606 | -31.674 | -0.068 | |
| Cl(5) | 2.757e-029 | | | | | |
| ClO3- | 2.757e-029 | 2.348e-029 | -28.560 | -28.629 | -0.070 | |
| Cl(7) | 1.527e-030 | | | | | |
| ClO4- | 1.526e-030 | 1.300e-030 | -29.816 | -29.886 | -0.070 | |
| ZnClO4+ | 8.875e-034 | 7.586e-034 | -33.052 | -33.120 | -0.068 | |
| Cu(1) | 8.770e-019 | | | | | |
| Cu+ | 8.101e-019 | 6.924e-019 | -18.091 | -18.160 | -0.068 | |
| CuCl2- | 6.618e-020 | 5.657e-020 | -19.179 | -19.247 | -0.068 | |
| CuCl3-2 | 7.615e-022 | 4.034e-022 | -21.118 | -21.394 | -0.276 | |
| Cu(2) | 3.356e-004 | | | | | |
| Cu+2 | 2.266e-004 | 1.265e-004 | -3.645 | -3.898 | -0.253 | |
| CuSO4 | 1.085e-004 | 1.085e-004 | -3.965 | -3.965 | 0.000 | |
| CuCl+ | 4.495e-007 | 3.842e-007 | -6.347 | -6.415 | -0.068 | |
| CuOH+ | 9.563e-009 | 8.174e-009 | -8.019 | -8.088 | -0.068 | |
| CuCl2 | 2.247e-010 | 2.247e-010 | -9.648 | -9.648 | 0.000 | |
| CuCl4-2 | 9.814e-021 | 5.199e-021 | -20.008 | -20.284 | -0.276 | |

| | | | | | |
|------------|------------|------------|---------|---------|--------|
| CuO2-2 | 2.089e-031 | 1.107e-031 | -30.680 | -30.956 | -0.276 |
| Fe(2) | 2.193e-008 | | | | |
| Fe+2 | 1.647e-008 | 9.190e-009 | -7.783 | -8.037 | -0.253 |
| FeSO4 | 5.453e-009 | 5.453e-009 | -8.263 | -8.263 | 0.000 |
| FeCl+ | 8.697e-012 | 7.434e-012 | -11.061 | -11.129 | -0.068 |
| FeOH+ | 4.259e-015 | 3.641e-015 | -14.371 | -14.439 | -0.068 |
| FeCl2 | 4.430e-017 | 4.430e-017 | -16.354 | -16.354 | 0.000 |
| FeCl4-2 | 2.980e-022 | 1.578e-022 | -21.526 | -21.802 | -0.276 |
| Fe(OH)2 | 3.623e-023 | 3.623e-023 | -22.441 | -22.441 | 0.000 |
| Fe(OH)3- | 2.114e-030 | 1.807e-030 | -29.675 | -29.743 | -0.068 |
| Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -41.369 | -41.645 | -0.276 |
| Fe(3) | 2.393e-003 | | | | |
| FeOH+2 | 1.327e-003 | 7.127e-004 | -2.877 | -3.147 | -0.270 |
| Fe(OH)2+ | 3.459e-004 | 2.956e-004 | -3.461 | -3.529 | -0.068 |
| Fe+3 | 2.843e-004 | 8.811e-005 | -3.546 | -4.055 | -0.509 |
| Fe2(OH)2+4 | 1.491e-004 | 1.367e-005 | -3.827 | -4.864 | -1.038 |
| FeSO4+ | 3.734e-005 | 3.192e-005 | -4.428 | -4.496 | -0.068 |
| Fe3(OH)4+5 | 3.276e-005 | 8.444e-007 | -4.485 | -6.073 | -1.589 |
| Fe(SO4)2- | 2.364e-006 | 2.021e-006 | -5.626 | -5.695 | -0.068 |
| Fe(OH)3 | 1.732e-007 | 1.732e-007 | -6.761 | -6.761 | 0.000 |
| FeCl+2 | 3.035e-008 | 1.630e-008 | -7.518 | -7.788 | -0.270 |
| FeCl2+ | 1.715e-008 | 1.466e-008 | -7.766 | -7.834 | -0.068 |
| Fe(OH)4- | 6.378e-014 | 5.452e-014 | -13.195 | -13.263 | -0.068 |
| FeCl4- | 2.542e-017 | 2.173e-017 | -16.595 | -16.663 | -0.068 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -43.299 | -43.296 | 0.003 |
| K | 7.759e-004 | | | | |
| K+ | 7.533e-004 | 6.391e-004 | -3.123 | -3.194 | -0.071 |
| KSO4- | 2.260e-005 | 1.932e-005 | -4.646 | -4.714 | -0.068 |
| KCl | 2.383e-008 | 2.383e-008 | -7.623 | -7.623 | 0.000 |
| KHSO4 | 1.360e-008 | 1.360e-008 | -7.866 | -7.866 | 0.000 |
| KOH | 2.776e-015 | 2.776e-015 | -14.557 | -14.557 | 0.000 |
| Mg | 3.543e-004 | | | | |
| Mg+2 | 2.237e-004 | 1.305e-004 | -3.650 | -3.884 | -0.234 |
| MgSO4 | 1.305e-004 | 1.305e-004 | -3.884 | -3.884 | 0.000 |
| MgCl+ | 1.323e-007 | 1.131e-007 | -6.878 | -6.946 | -0.068 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -41.859 | -42.896 | -1.038 |
| Mn(2) | 2.570e-004 | | | | |
| Mn+2 | 1.694e-004 | 9.453e-005 | -3.771 | -4.024 | -0.253 |
| MnSO4 | 8.733e-005 | 8.733e-005 | -4.059 | -4.059 | 0.000 |
| MnCl+ | 2.615e-007 | 2.235e-007 | -6.583 | -6.651 | -0.068 |
| MnOH+ | 3.561e-012 | 3.044e-012 | -11.448 | -11.517 | -0.068 |
| MnCl3- | 7.044e-014 | 6.021e-014 | -13.152 | -13.220 | -0.068 |
| Mn2OH+3 | 1.215e-015 | 3.083e-016 | -14.915 | -15.511 | -0.596 |
| Mn(OH)2 | 9.361e-021 | 9.361e-021 | -20.029 | -20.029 | 0.000 |
| Mn2(OH)3+ | 2.588e-023 | 2.212e-023 | -22.587 | -22.655 | -0.068 |
| Mn(OH)3- | 1.287e-029 | 1.100e-029 | -28.890 | -28.959 | -0.068 |
| Mn(OH)4-2 | 2.203e-040 | 1.167e-040 | -39.657 | -39.933 | -0.276 |
| Mn(3) | 9.938e-013 | | | | |
| Mn+3 | 9.938e-013 | 2.521e-013 | -12.003 | -12.598 | -0.596 |
| Mn(6) | 3.873e-030 | | | | |
| MnO4-2 | 3.873e-030 | 2.052e-030 | -29.412 | -29.688 | -0.276 |
| Mn(7) | 1.061e-022 | | | | |
| MnO4- | 1.061e-022 | 9.036e-023 | -21.974 | -22.044 | -0.070 |
| Na | 8.492e-004 | | | | |
| Na+ | 8.286e-004 | 7.083e-004 | -3.082 | -3.150 | -0.068 |
| NaSO4- | 2.050e-005 | 1.752e-005 | -4.688 | -4.756 | -0.068 |
| NaCl | 1.382e-007 | 1.382e-007 | -6.859 | -6.859 | 0.000 |
| NaOH | 1.475e-015 | 1.475e-015 | -14.831 | -14.831 | 0.000 |
| NaAlO2 | 2.057e-019 | 2.057e-019 | -18.687 | -18.687 | 0.000 |
| O(0) | 4.953e-006 | | | | |
| O2 | 2.476e-006 | 2.493e-006 | -5.606 | -5.603 | 0.003 |
| S(6) | 8.652e-003 | | | | |
| SO4-2 | 7.068e-003 | 3.744e-003 | -2.151 | -2.427 | -0.276 |
| CaSO4 | 4.580e-004 | 4.580e-004 | -3.339 | -3.339 | 0.000 |
| HSO4- | 3.531e-004 | 3.018e-004 | -3.452 | -3.520 | -0.068 |
| AlSO4+ | 2.135e-004 | 1.825e-004 | -3.671 | -3.739 | -0.068 |

| | | | | | |
|-----------|------------|------------|---------|---------|--------|
| MgSO4 | 1.305e-004 | 1.305e-004 | -3.884 | -3.884 | 0.000 |
| CuSO4 | 1.085e-004 | 1.085e-004 | -3.965 | -3.965 | 0.000 |
| MnSO4 | 8.733e-005 | 8.733e-005 | -4.059 | -4.059 | 0.000 |
| Al(SO4)2- | 6.205e-005 | 5.304e-005 | -4.207 | -4.275 | -0.068 |
| FeSO4+ | 3.734e-005 | 3.192e-005 | -4.428 | -4.496 | -0.068 |
| ZnSO4 | 2.427e-005 | 2.427e-005 | -4.615 | -4.615 | 0.000 |
| KSO4- | 2.260e-005 | 1.932e-005 | -4.646 | -4.714 | -0.068 |
| NaSO4- | 2.050e-005 | 1.752e-005 | -4.688 | -4.756 | -0.068 |
| Fe(SO4)2- | 2.364e-006 | 2.021e-006 | -5.626 | -5.695 | -0.068 |
| KHSO4 | 1.360e-008 | 1.360e-008 | -7.866 | -7.866 | 0.000 |
| FeSO4 | 5.453e-009 | 5.453e-009 | -8.263 | -8.263 | 0.000 |
| H2SO4 | 2.272e-010 | 2.272e-010 | -9.644 | -9.644 | 0.000 |
| Zn | 7.962e-005 | | | | |
| Zn+2 | 5.528e-005 | 3.085e-005 | -4.257 | -4.511 | -0.253 |
| ZnSO4 | 2.427e-005 | 2.427e-005 | -4.615 | -4.615 | 0.000 |
| ZnCl+ | 6.734e-008 | 5.756e-008 | -7.172 | -7.240 | -0.068 |
| ZnCl2 | 7.466e-011 | 7.466e-011 | -10.127 | -10.127 | 0.000 |
| ZnOH+ | 4.959e-011 | 4.239e-011 | -10.305 | -10.373 | -0.068 |
| Zn(OH)Cl | 1.233e-012 | 1.233e-012 | -11.909 | -11.909 | 0.000 |
| ZnCl3- | 5.357e-014 | 4.579e-014 | -13.271 | -13.339 | -0.068 |
| ZnCl4-2 | 7.275e-016 | 3.854e-016 | -15.138 | -15.414 | -0.276 |
| Zn(OH)2 | 2.274e-016 | 2.274e-016 | -15.643 | -15.643 | 0.000 |
| Zn(OH)3- | 1.033e-024 | 8.831e-025 | -23.986 | -24.054 | -0.068 |
| ZnClO4+ | 8.875e-034 | 7.586e-034 | -33.052 | -33.120 | -0.068 |
| Zn(OH)4-2 | 3.560e-034 | 1.886e-034 | -33.448 | -33.724 | -0.276 |

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

| Phase | SI | log IAP | log KT | |
|-------------------|---------|---------|--------|-------------------|
| Al | -140.74 | 9.17 | 149.91 | Al |
| Al(g) | -191.44 | 9.17 | 200.62 | Al |
| Al2(SO4)3 | -34.82 | -15.92 | 18.90 | Al2(SO4)3 |
| Al2(SO4)3:6H2O | -17.48 | -15.92 | 1.56 | Al2(SO4)3:6H2O |
| Alum-K | -7.40 | -12.37 | -4.97 | KAl(SO4)2:12H2O |
| Alunite | -1.96 | -2.43 | -0.47 | KAl3(OH)6(SO4)2 |
| Anhydrite | -1.15 | -5.50 | -4.35 | CaSO4 |
| Antarcticite | -13.08 | -8.99 | 4.09 | CaCl2:6H2O |
| Antlerite | -10.46 | -1.73 | 8.73 | Cu3(SO4)(OH)4 |
| Aphthitalite | -13.70 | -17.59 | -3.89 | NaK3(SO4)2 |
| Arcanite | -6.97 | -8.82 | -1.84 | K2SO4 |
| Arsenolite | -51.34 | -71.18 | -19.84 | As2O3 |
| As | -74.07 | -31.39 | 42.68 | As |
| As2O5 | -17.85 | -15.72 | 2.14 | As2O5 |
| As4O6(cubi) | -102.53 | -142.36 | -39.82 | As4O6 |
| As4O6(mono) | -102.31 | -142.36 | -40.05 | As4O6 |
| Atacamite | -17.18 | -2.91 | 14.26 | Cu4Cl2(OH)6 |
| Bassanite | -1.80 | -5.50 | -3.71 | CaSO4:0.5H2O |
| Birnessite | -11.25 | -96.79 | -85.55 | Mn8O14:5H2O |
| Bischofite | -14.19 | -9.79 | 4.39 | MgCl2:6H2O |
| Bixbyite | -5.64 | -6.61 | -0.96 | Mn2O3 |
| Bloedite | -12.56 | -15.04 | -2.48 | Na2Mg(SO4)2:4H2O |
| Boehmite | -2.58 | 4.97 | 7.55 | AlO2H |
| Brochantite | -14.85 | 0.57 | 15.42 | Cu4(SO4)(OH)6 |
| Brucite | -13.97 | 2.31 | 16.28 | Mg(OH)2 |
| Ca | -133.91 | 5.92 | 139.83 | Ca |
| Ca(g) | -159.15 | 5.92 | 165.07 | Ca |
| Ca2Al2O5:8H2O | -43.39 | 16.18 | 59.57 | Ca2Al2O5:8H2O |
| Ca2Cl2(OH)2:H2O | -32.16 | -5.87 | 26.29 | Ca2Cl2(OH)2:H2O |
| Ca3(AsO4)2 | -24.16 | -6.36 | 17.80 | Ca3(AsO4)2 |
| Ca3Al2O6 | -93.73 | 19.30 | 113.03 | Ca3Al2O6 |
| Ca4Al2Fe2O10 | -107.59 | 32.90 | 140.48 | Ca4Al2Fe2O10 |
| Ca4Al2O7:13H2O | -84.84 | 22.42 | 107.25 | Ca4Al2O7:13H2O |
| Ca4Al2O7:19H2O | -81.27 | 22.42 | 103.68 | Ca4Al2O7:19H2O |
| Ca4Cl2(OH)6:13H2O | -67.96 | 0.37 | 68.33 | Ca4Cl2(OH)6:13H2O |
| CaAl2O4 | -33.85 | 13.06 | 46.91 | CaAl2O4 |
| CaAl2O4:10H2O | -24.93 | 13.06 | 37.99 | CaAl2O4:10H2O |

| | | | | |
|-------------------------|---------|--------|--------|--------------------------|
| CaAl4O7 | -45.59 | 23.01 | 68.59 | CaAl4O7 |
| Carnallite | -20.22 | -15.94 | 4.27 | KMgCl3:6H2O |
| CaSO4:0.5H2O(beta) | -1.97 | -5.50 | -3.54 | CaSO4:0.5H2O |
| Chalcanthite | -3.70 | -6.33 | -2.63 | CuSO4:5H2O |
| Chalcocyanite | -9.24 | -6.32 | 2.91 | CuSO4 |
| Chloromagnesite | -31.61 | -9.79 | 21.82 | MgCl2 |
| Cl2(g) | -17.90 | -14.91 | 2.99 | Cl2 |
| Claudetite | -51.38 | -71.18 | -19.80 | As2O3 |
| Corundum | -8.35 | 9.94 | 18.29 | Al2O3 |
| Cu | -26.40 | 5.10 | 31.50 | Cu |
| Cu(g) | -78.56 | 5.10 | 83.66 | Cu |
| CuCl2 | -13.53 | -9.81 | 3.72 | CuCl2 |
| Cuprite | -28.22 | -30.12 | -1.91 | Cu2O |
| Delafossite | -3.39 | -9.82 | -6.44 | CuFeO2 |
| Diaspore | -2.17 | 4.97 | 7.15 | AlHO2 |
| Epsomite | -4.35 | -6.31 | -1.96 | MgSO4:7H2O |
| Ettringite | -59.68 | 2.78 | 62.46 | Ca6Al2(SO4)3(OH)12:26H2O |
| Fe | -58.06 | 0.96 | 59.02 | Fe |
| Fe(OH)2 | -15.74 | -1.84 | 13.89 | Fe(OH)2 |
| Fe(OH)3 | -0.40 | 5.24 | 5.64 | Fe(OH)3 |
| Fe2(SO4)3 | -18.44 | -15.39 | 3.05 | Fe2(SO4)3 |
| FeO | -15.36 | -1.84 | 13.52 | FeO |
| Ferrite-Ca | -7.90 | 13.60 | 21.50 | CaFe2O4 |
| Ferrite-Cu | 2.49 | 12.78 | 10.28 | CuFe2O4 |
| Ferrite-Dicalcium | -40.08 | 16.72 | 56.80 | Ca2Fe2O5 |
| Ferrite-Mg | -8.23 | 12.79 | 21.02 | MgFe2O4 |
| Ferrite-Zn | 0.46 | 12.16 | 11.70 | ZnFe2O4 |
| FeSO4 | -13.07 | -10.46 | 2.61 | FeSO4 |
| Gibbsite | -2.77 | 4.97 | 7.74 | Al(OH)3 |
| Glauberite | -8.76 | -14.23 | -5.47 | Na2Ca(SO4)2 |
| Goethite | 4.71 | 5.24 | 0.53 | FeOOH |
| Gypsum | -0.97 | -5.50 | -4.53 | CaSO4:2H2O |
| H2(g) | -40.20 | -43.30 | -3.10 | H2 |
| H2O(g) | -1.59 | -0.00 | 1.59 | H2O |
| Halite | -7.67 | -6.10 | 1.56 | NaCl |
| Hausmannite | -14.58 | -4.44 | 10.14 | Mn3O4 |
| HCl(g) | -12.35 | -6.05 | 6.30 | HCl |
| Hematite | 10.40 | 10.48 | 0.08 | Fe2O3 |
| Hercynite | -20.70 | 8.10 | 28.80 | FeAl2O4 |
| Hexahydrite | -4.59 | -6.31 | -1.73 | MgSO4:6H2O |
| Hydrophilite | -20.73 | -8.99 | 11.75 | CaCl2 |
| Ice | -0.14 | -0.00 | 0.14 | H2O |
| Jarosite | 7.79 | -1.63 | -9.41 | KFe3(SO4)2(OH)6 |
| Jarosite-Na | 3.87 | -1.58 | -5.45 | NaFe3(SO4)2(OH)6 |
| K | -69.67 | 1.30 | 70.98 | K |
| K(g) | -80.27 | 1.30 | 81.58 | K |
| K2O | -84.23 | -0.19 | 84.04 | K2O |
| K3H(SO4)2 | -13.91 | -17.53 | -3.62 | K3H(SO4)2 |
| Kainite | -12.15 | -12.46 | -0.31 | KMgClSO4:3H2O |
| KAl(SO4)2 | -15.64 | -12.37 | 3.27 | KAl(SO4)2 |
| Katoite | -59.64 | 19.30 | 78.94 | Ca3Al2H12O12 |
| Kieserite | -6.04 | -6.31 | -0.27 | MgSO4:H2O |
| KMgCl3 | -37.19 | -15.94 | 21.25 | KMgCl3 |
| KMgCl3:2H2O | -29.90 | -15.94 | 13.96 | KMgCl3:2H2O |
| Lammerite | -10.38 | -8.82 | 1.55 | Cu3(AsO4)2 |
| Lawrencite | -23.00 | -13.95 | 9.05 | FeCl2 |
| Leonite | -11.01 | -15.13 | -4.11 | K2Mg(SO4)2:4H2O |
| Lime | -29.45 | 3.12 | 32.57 | CaO |
| Magnetite | -1.78 | 8.64 | 10.42 | Fe3O4 |
| Manganite | -3.14 | -3.30 | -0.16 | MnO(OH) |
| Manganosite | -15.74 | 2.17 | 17.92 | MnO |
| Mayenite | -387.12 | 107.03 | 494.15 | Ca12Al14O33 |
| Melanterite | -8.07 | -10.46 | -2.40 | FeSO4:7H2O |
| Mercallite | -7.28 | -8.72 | -1.44 | KHSO4 |
| Mg | -117.41 | 5.11 | 122.52 | Mg |
| Mg(g) | -137.13 | 5.11 | 142.25 | Mg |
| Mg1.25SO4(OH)0.5:0.5H2O | -10.93 | -5.73 | 5.20 | Mg1.25SO4(OH)0.5:0.5H2O |

| | | | | |
|------------------|--------|--------|--------|--------------------|
| Mg1.5SO4(OH) | -14.36 | -5.16 | 9.21 | Mg1.5SO4(OH) |
| MgCl2:2H2O | -22.53 | -9.79 | 12.73 | MgCl2:2H2O |
| MgCl2:4H2O | -17.10 | -9.79 | 7.30 | MgCl2:4H2O |
| MgCl2:H2O | -25.87 | -9.79 | 16.07 | MgCl2:H2O |
| MgOHCl | -19.63 | -3.74 | 15.89 | MgOHCl |
| MgSO4 | -11.14 | -6.31 | 4.83 | MgSO4 |
| Mirabilite | -7.57 | -8.73 | -1.15 | Na2SO4:10H2O |
| Misenite | -50.05 | -61.13 | -11.08 | K8H6(SO4)7 |
| Mn | -77.96 | 4.97 | 82.93 | Mn |
| Mn(OH)2(am) | -13.14 | 2.17 | 15.31 | Mn(OH)2 |
| Mn(OH)3 | -9.65 | -3.30 | 6.34 | Mn(OH)3 |
| MnCl2:2H2O | -13.93 | -9.93 | 4.00 | MnCl2:2H2O |
| MnCl2:4H2O | -12.69 | -9.93 | 2.75 | MnCl2:4H2O |
| MnCl2:H2O | -15.48 | -9.93 | 5.54 | MnCl2:H2O |
| MnO2(gamma) | -0.73 | -16.86 | -16.13 | MnO2 |
| MnSO4 | -9.06 | -6.45 | 2.61 | MnSO4 |
| Molysite | -26.39 | -12.92 | 13.47 | FeCl3 |
| Na | -66.02 | 1.35 | 67.37 | Na |
| Na(g) | -79.51 | 1.35 | 80.86 | Na |
| Na2O | -67.52 | -0.10 | 67.42 | Na2O |
| Na3H(SO4)2 | -16.51 | -17.40 | -0.89 | Na3H(SO4)2 |
| Na4Ca(SO4)3:2H2O | -17.06 | -22.96 | -5.89 | Na4Ca(SO4)3:2H2O |
| NaFeO2 | -14.70 | 5.19 | 19.88 | NaFeO2 |
| Nantokite | -14.35 | -21.11 | -6.77 | CuCl |
| O2(g) | -2.71 | -5.60 | -2.89 | O2 |
| Oxychloride-Mg | -27.26 | -1.43 | 25.83 | Mg2Cl(OH)3:4H2O |
| Pentahydrate | -4.92 | -6.31 | -1.39 | MgSO4:5H2O |
| Periclase | -19.01 | 2.31 | 21.33 | MgO |
| Picromerite | -10.69 | -15.13 | -4.44 | K2Mg(SO4)2:6H2O |
| Polyhalite | -11.82 | -26.13 | -14.31 | K2MgCa2(SO4)4:2H2O |
| Portlandite | -19.43 | 3.12 | 22.55 | Ca(OH)2 |
| Pyrolusite | 0.80 | -16.86 | -17.66 | MnO2 |
| Scacchite | -18.67 | -9.93 | 8.74 | MnCl2 |
| Spinel | -25.35 | 12.25 | 37.61 | Al2MgO4 |
| Starkeyite | -5.31 | -6.31 | -1.00 | MgSO4:4H2O |
| Sylvite | -6.98 | -6.15 | 0.83 | KCl |
| Syngenite | -6.72 | -14.32 | -7.60 | K2Ca(SO4)2:H2O |
| Tachyhydrate | -45.72 | -28.57 | 17.14 | Mg2CaCl6:12H2O |
| Tenorite | -5.35 | 2.30 | 7.65 | CuO |
| Thenardite | -8.37 | -8.73 | -0.36 | Na2SO4 |
| Todorokite | -9.89 | -55.71 | -45.82 | Mn7O12:3H2O |
| Wustite | -13.40 | -0.99 | 12.40 | Fe.9470 |
| Zincite | -9.51 | 1.69 | 11.20 | ZnO |
| Zn | -64.30 | 4.49 | 68.79 | Zn |
| Zn(ClO4)2:6H2O | -69.92 | -64.28 | 5.63 | Zn(ClO4)2:6H2O |
| Zn(g) | -80.92 | 4.49 | 85.41 | Zn |
| Zn(OH)2(beta) | -10.25 | 1.69 | 11.93 | Zn(OH)2 |
| Zn(OH)2(epsilon) | -9.98 | 1.69 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -10.20 | 1.69 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -17.97 | -2.68 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -12.83 | -5.25 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -19.97 | -10.66 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -31.28 | -12.19 | 19.09 | Zn3O(SO4)2 |
| ZnCl2 | -17.50 | -10.42 | 7.08 | ZnCl2 |
| ZnSO4 | -10.47 | -6.94 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -5.24 | -6.94 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -5.06 | -6.94 | -1.88 | ZnSO4:7H2O |
| ZnSO4:H2O | -6.39 | -6.94 | -0.55 | ZnSO4:H2O |

Initial solution 2. Inter 3

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

| Elements | Molality | Moles |
|----------|------------|------------|
| Al | 1.284e-003 | 1.284e-003 |
| As | 1.337e-007 | 1.337e-007 |

| | | |
|------|------------|------------|
| Ca | 7.623e-003 | 7.623e-003 |
| Cl | 1.105e-003 | 1.105e-003 |
| Cu | 2.049e-006 | 2.049e-006 |
| Fe | 2.181e-004 | 2.181e-004 |
| K | 2.221e-004 | 2.221e-004 |
| Mg | 1.223e-003 | 1.223e-003 |
| Mn | 2.547e-004 | 2.547e-004 |
| Na | 2.843e-003 | 2.843e-003 |
| S(6) | 1.161e-002 | 1.161e-002 |
| Zn | 3.064e-007 | 3.064e-007 |

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

| | | |
|--|---|---------------|
| pH | = | 2.290 |
| pe | = | 12.000 |
| Activity of water | = | 1.000 |
| Ionic strength | = | 3.680e-002 |
| Mass of water (kg) | = | 1.000e+000 |
| Total alkalinity (eq/kg) | = | -7.977e-003 |
| Total carbon (mol/kg) | = | 0.000e+000 |
| Total CO2 (mol/kg) | = | 0.000e+000 |
| Temperature (deg C) | = | 25.000 |
| Electrical balance (eq) | = | 9.172e-003 |
| Percent error, 100*(Cat- An)/(Cat+ An) | = | 21.65 |
| Iterations | = | 8 |
| Total H | = | 1.110586e+002 |
| Total O | = | 5.557178e+001 |

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|----------------|------------|------------|--------------|--------------|-----------|
| H+ | 5.903e-003 | 5.129e-003 | -2.229 | -2.290 | -0.061 |
| OH- | 2.252e-012 | 1.878e-012 | -11.648 | -11.726 | -0.079 |
| H2O | 5.553e+001 | 9.995e-001 | 1.744 | -0.000 | 0.000 |
| Al | 1.284e-003 | | | | |
| AlSO4+ | 5.907e-004 | 4.949e-004 | -3.229 | -3.305 | -0.077 |
| Al+3 | 5.446e-004 | 1.494e-004 | -3.264 | -3.826 | -0.562 |
| Al(SO4)2- | 1.484e-004 | 1.244e-004 | -3.828 | -3.905 | -0.077 |
| AlOH+2 | 6.571e-007 | 3.262e-007 | -6.182 | -6.487 | -0.304 |
| Al2(OH)2+4 | 2.524e-010 | 1.730e-011 | -9.598 | -10.762 | -1.164 |
| Al(OH)2+ | 1.762e-010 | 1.476e-010 | -9.754 | -9.831 | -0.077 |
| HALO2 | 4.189e-014 | 4.189e-014 | -13.378 | -13.378 | 0.000 |
| Al3(OH)4+5 | 3.800e-015 | 6.338e-017 | -14.420 | -16.198 | -1.778 |
| AlO2- | 3.339e-018 | 2.798e-018 | -17.476 | -17.553 | -0.077 |
| NaAlO2 | 1.245e-021 | 1.245e-021 | -20.905 | -20.905 | 0.000 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -71.703 | -75.189 | -3.486 |
| As(-3) | 0.000e+000 | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -107.015 | -107.015 | 0.000 |
| As(3) | 8.809e-017 | | | | |
| HAsO2 | 4.701e-017 | 4.701e-017 | -16.328 | -16.328 | 0.000 |
| As(OH)3 | 4.108e-017 | 4.108e-017 | -16.386 | -16.386 | 0.000 |
| H2AsO3- | 5.847e-024 | 4.899e-024 | -23.233 | -23.310 | -0.077 |
| AsO2- | 5.592e-024 | 4.686e-024 | -23.252 | -23.329 | -0.077 |
| AsO2OH-2 | 1.914e-032 | 9.333e-033 | -31.718 | -32.030 | -0.312 |
| As(5) | 1.337e-007 | | | | |
| H2AsO4- | 7.609e-008 | 6.375e-008 | -7.119 | -7.195 | -0.077 |
| H3AsO4 | 5.759e-008 | 5.759e-008 | -7.240 | -7.240 | 0.000 |
| HAsO4-2 | 4.231e-012 | 2.064e-012 | -11.374 | -11.685 | -0.312 |
| AsO4-3 | 5.216e-021 | 1.032e-021 | -20.283 | -20.986 | -0.704 |
| Ca | 7.623e-003 | | | | |
| Ca+2 | 6.115e-003 | 3.186e-003 | -2.214 | -2.497 | -0.283 |
| CaSO4 | 1.507e-003 | 1.507e-003 | -2.822 | -2.822 | 0.000 |
| CaCl+ | 7.369e-007 | 6.174e-007 | -6.133 | -6.209 | -0.077 |
| CaCl2 | 6.641e-010 | 6.641e-010 | -9.178 | -9.178 | 0.000 |
| CaOH+ | 1.047e-013 | 8.770e-014 | -12.980 | -13.057 | -0.077 |

| | | | | | | |
|------------|------------|------------|---------|---------|--------|--|
| Cl(-1) | 1.105e-003 | | | | | |
| Cl- | 1.102e-003 | 9.144e-004 | -2.958 | -3.039 | -0.081 | |
| HCl | 1.053e-006 | 1.053e-006 | -5.977 | -5.977 | 0.000 | |
| CaCl+ | 7.369e-007 | 6.174e-007 | -6.133 | -6.209 | -0.077 | |
| MgCl+ | 3.884e-007 | 3.254e-007 | -6.411 | -6.488 | -0.077 | |
| NaCl | 3.748e-007 | 3.748e-007 | -6.426 | -6.426 | 0.000 | |
| MnCl+ | 2.176e-007 | 1.823e-007 | -6.662 | -6.739 | -0.077 | |
| FeCl+ | 5.641e-008 | 4.726e-008 | -7.249 | -7.325 | -0.077 | |
| KCl | 5.516e-009 | 5.516e-009 | -8.258 | -8.258 | 0.000 | |
| CuCl+ | 2.296e-009 | 1.924e-009 | -8.639 | -8.716 | -0.077 | |
| FeCl+2 | 2.088e-009 | 1.036e-009 | -8.680 | -8.984 | -0.304 | |
| FeCl2+ | 9.157e-010 | 7.673e-010 | -9.038 | -9.115 | -0.077 | |
| CaCl2 | 6.641e-010 | 6.641e-010 | -9.178 | -9.178 | 0.000 | |
| ZnCl+ | 2.159e-010 | 1.809e-010 | -9.666 | -9.743 | -0.077 | |
| CuCl2 | 9.263e-013 | 9.263e-013 | -12.033 | -12.033 | 0.000 | |
| FeCl2 | 2.319e-013 | 2.319e-013 | -12.635 | -12.635 | 0.000 | |
| ZnCl2 | 1.932e-013 | 1.932e-013 | -12.714 | -12.714 | 0.000 | |
| MnCl3- | 3.974e-014 | 3.329e-014 | -13.401 | -13.478 | -0.077 | |
| Zn(OH)Cl | 6.029e-016 | 6.029e-016 | -15.220 | -15.220 | 0.000 | |
| ZnCl3- | 1.165e-016 | 9.758e-017 | -15.934 | -16.011 | -0.077 | |
| CuCl2- | 2.784e-017 | 2.332e-017 | -16.555 | -16.632 | -0.077 | |
| ZnCl4-2 | 1.387e-018 | 6.763e-019 | -17.858 | -18.170 | -0.312 | |
| FeCl4-2 | 1.149e-018 | 5.603e-019 | -17.940 | -18.252 | -0.312 | |
| FeCl4- | 9.205e-019 | 7.713e-019 | -18.036 | -18.113 | -0.077 | |
| CuCl3-2 | 2.809e-019 | 1.370e-019 | -18.552 | -18.863 | -0.312 | |
| CuCl4-2 | 2.980e-023 | 1.454e-023 | -22.526 | -22.838 | -0.312 | |
| Cl(1) | 5.148e-028 | | | | | |
| HClO | 5.148e-028 | 5.148e-028 | -27.288 | -27.288 | 0.000 | |
| ClO- | 3.230e-033 | 2.707e-033 | -32.491 | -32.568 | -0.077 | |
| Cl(3) | 0.000e+000 | | | | | |
| HClO2 | 0.000e+000 | 0.000e+000 | -54.111 | -54.111 | 0.000 | |
| ClO2- | 0.000e+000 | 0.000e+000 | -54.914 | -54.991 | -0.077 | |
| Cl(5) | 0.000e+000 | | | | | |
| ClO3- | 0.000e+000 | 0.000e+000 | -63.483 | -63.562 | -0.079 | |
| Cl(7) | 0.000e+000 | | | | | |
| ClO4- | 0.000e+000 | 0.000e+000 | -76.356 | -76.435 | -0.079 | |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -82.010 | -82.087 | -0.077 | |
| Cu(1) | 5.307e-016 | | | | | |
| Cu+ | 5.025e-016 | 4.211e-016 | -15.299 | -15.376 | -0.077 | |
| CuCl2- | 2.784e-017 | 2.332e-017 | -16.555 | -16.632 | -0.077 | |
| CuCl3-2 | 2.809e-019 | 1.370e-019 | -18.552 | -18.863 | -0.312 | |
| Cu(2) | 2.049e-006 | | | | | |
| Cu+2 | 1.476e-006 | 7.692e-007 | -5.831 | -6.114 | -0.283 | |
| CuSO4 | 5.704e-007 | 5.704e-007 | -6.244 | -6.244 | 0.000 | |
| CuCl+ | 2.296e-009 | 1.924e-009 | -8.639 | -8.716 | -0.077 | |
| CuOH+ | 9.229e-012 | 7.732e-012 | -11.035 | -11.112 | -0.077 | |
| CuCl2 | 9.263e-013 | 9.263e-013 | -12.033 | -12.033 | 0.000 | |
| CuCl4-2 | 2.980e-023 | 1.454e-023 | -22.526 | -22.838 | -0.312 | |
| CuO2-2 | 8.086e-037 | 3.944e-037 | -36.092 | -36.404 | -0.312 | |
| Fe(2) | 1.726e-004 | | | | | |
| Fe+2 | 1.362e-004 | 7.095e-005 | -3.866 | -4.149 | -0.283 | |
| FeSO4 | 3.640e-005 | 3.640e-005 | -4.439 | -4.439 | 0.000 | |
| FeCl+ | 5.641e-008 | 4.726e-008 | -7.249 | -7.325 | -0.077 | |
| FeOH+ | 5.219e-012 | 4.373e-012 | -11.282 | -11.359 | -0.077 | |
| FeCl2 | 2.319e-013 | 2.319e-013 | -12.635 | -12.635 | 0.000 | |
| FeCl4-2 | 1.149e-018 | 5.603e-019 | -17.940 | -18.252 | -0.312 | |
| Fe(OH)2 | 6.769e-021 | 6.769e-021 | -20.169 | -20.169 | 0.000 | |
| Fe(OH)3- | 6.268e-029 | 5.252e-029 | -28.203 | -28.280 | -0.077 | |
| Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -40.678 | -40.990 | -0.312 | |
| Fe(3) | 4.544e-005 | | | | | |
| Fe+3 | 2.480e-005 | 6.803e-006 | -4.606 | -5.167 | -0.562 | |
| FeOH+2 | 1.724e-005 | 8.560e-006 | -4.763 | -5.068 | -0.304 | |
| FeSO4+ | 2.543e-006 | 2.131e-006 | -5.595 | -5.671 | -0.077 | |
| Fe(OH)2+ | 6.593e-007 | 5.524e-007 | -6.181 | -6.258 | -0.077 | |
| Fe(SO4)2- | 1.392e-007 | 1.166e-007 | -6.856 | -6.933 | -0.077 | |
| Fe2(OH)2+4 | 2.876e-008 | 1.972e-009 | -7.541 | -8.705 | -1.164 | |
| FeCl+2 | 2.088e-009 | 1.036e-009 | -8.680 | -8.984 | -0.304 | |

| | | | | | | |
|-------|-------------------------------------|------------|------------|---------|---------|--------|
| | FeCl ₂ + | 9.157e-010 | 7.673e-010 | -9.038 | -9.115 | -0.077 |
| | Fe(OH) ₃ | 5.035e-011 | 5.035e-011 | -10.298 | -10.298 | 0.000 |
| | Fe ₃ (OH) ₄₊₅ | 1.365e-011 | 2.276e-013 | -10.865 | -12.643 | -1.778 |
| | Fe(OH) ₄₋ | 2.942e-018 | 2.465e-018 | -17.531 | -17.608 | -0.077 |
| | FeCl ₄₋ | 9.205e-019 | 7.713e-019 | -18.036 | -18.113 | -0.077 |
| H(0) | | 4.137e-032 | | | | |
| | H ₂ | 2.069e-032 | 2.087e-032 | -31.684 | -31.680 | 0.004 |
| K | | 2.221e-004 | | | | |
| | K+ | 2.165e-004 | 1.797e-004 | -3.665 | -3.746 | -0.081 |
| | KSO ₄₋ | 5.603e-006 | 4.694e-006 | -5.252 | -5.328 | -0.077 |
| | KHSO ₄ | 2.124e-008 | 2.124e-008 | -7.673 | -7.673 | 0.000 |
| | KCl | 5.516e-009 | 5.516e-009 | -8.258 | -8.258 | 0.000 |
| | KOH | 1.214e-016 | 1.214e-016 | -15.916 | -15.916 | 0.000 |
| Mg | | 1.223e-003 | | | | |
| | Mg+2 | 8.282e-004 | 4.559e-004 | -3.082 | -3.341 | -0.259 |
| | MgSO ₄ | 3.941e-004 | 3.941e-004 | -3.404 | -3.404 | 0.000 |
| | MgCl+ | 3.884e-007 | 3.254e-007 | -6.411 | -6.488 | -0.077 |
| | Mg ₄ (OH) ₄₊₄ | 0.000e+000 | 0.000e+000 | -42.792 | -43.955 | -1.164 |
| Mn(2) | | 2.547e-004 | | | | |
| | Mn+2 | 1.797e-004 | 9.362e-005 | -3.745 | -4.029 | -0.283 |
| | MnSO ₄ | 7.478e-005 | 7.478e-005 | -4.126 | -4.126 | 0.000 |
| | MnCl+ | 2.176e-007 | 1.823e-007 | -6.662 | -6.739 | -0.077 |
| | MnOH+ | 5.598e-013 | 4.690e-013 | -12.252 | -12.329 | -0.077 |
| | MnCl ₃₋ | 3.974e-014 | 3.329e-014 | -13.401 | -13.478 | -0.077 |
| | Mn ₂ OH+3 | 2.199e-016 | 4.705e-017 | -15.658 | -16.327 | -0.670 |
| | Mn(OH) ₂ | 2.244e-022 | 2.244e-022 | -21.649 | -21.649 | 0.000 |
| | Mn ₂ (OH) ₃₊ | 9.749e-026 | 8.168e-026 | -25.011 | -25.088 | -0.077 |
| | Mn(OH) ₃₋ | 4.895e-032 | 4.101e-032 | -31.310 | -31.387 | -0.077 |
| | Mn(OH) ₄₋₂ | 0.000e+000 | 0.000e+000 | -42.858 | -43.169 | -0.312 |
| Mn(3) | | 1.167e-017 | | | | |
| | Mn+3 | 1.167e-017 | 2.497e-018 | -16.933 | -17.603 | -0.670 |
| Mn(6) | | 0.000e+000 | | | | |
| | MnO ₄₋₂ | 0.000e+000 | 0.000e+000 | -55.845 | -56.156 | -0.312 |
| Mn(7) | | 0.000e+000 | | | | |
| | MnO ₄₋ | 0.000e+000 | 0.000e+000 | -53.434 | -53.513 | -0.079 |
| Na | | 2.843e-003 | | | | |
| | Na+ | 2.783e-003 | 2.332e-003 | -2.555 | -2.632 | -0.077 |
| | NaSO ₄₋ | 5.953e-005 | 4.988e-005 | -4.225 | -4.302 | -0.077 |
| | NaCl | 3.748e-007 | 3.748e-007 | -6.426 | -6.426 | 0.000 |
| | NaOH | 7.555e-016 | 7.555e-016 | -15.122 | -15.122 | 0.000 |
| | NaAlO ₂ | 1.245e-021 | 1.245e-021 | -20.905 | -20.905 | 0.000 |
| O(0) | | 2.895e-029 | | | | |
| | O ₂ | 1.448e-029 | 1.460e-029 | -28.839 | -28.836 | 0.004 |
| S(6) | | 1.161e-002 | | | | |
| | SO ₄₋₂ | 6.638e-003 | 3.237e-003 | -2.178 | -2.490 | -0.312 |
| | HSO ₄₋ | 2.002e-003 | 1.677e-003 | -2.699 | -2.775 | -0.077 |
| | CaSO ₄ | 1.507e-003 | 1.507e-003 | -2.822 | -2.822 | 0.000 |
| | AlSO ₄₊ | 5.907e-004 | 4.949e-004 | -3.229 | -3.305 | -0.077 |
| | MgSO ₄ | 3.941e-004 | 3.941e-004 | -3.404 | -3.404 | 0.000 |
| | Al(SO ₄) ₂₋ | 1.484e-004 | 1.244e-004 | -3.828 | -3.905 | -0.077 |
| | MnSO ₄ | 7.478e-005 | 7.478e-005 | -4.126 | -4.126 | 0.000 |
| | NaSO ₄₋ | 5.953e-005 | 4.988e-005 | -4.225 | -4.302 | -0.077 |
| | FeSO ₄ | 3.640e-005 | 3.640e-005 | -4.439 | -4.439 | 0.000 |
| | KSO ₄₋ | 5.603e-006 | 4.694e-006 | -5.252 | -5.328 | -0.077 |
| | FeSO ₄₊ | 2.543e-006 | 2.131e-006 | -5.595 | -5.671 | -0.077 |
| | CuSO ₄ | 5.704e-007 | 5.704e-007 | -6.244 | -6.244 | 0.000 |
| | Fe(SO ₄) ₂₋ | 1.392e-007 | 1.166e-007 | -6.856 | -6.933 | -0.077 |
| | ZnSO ₄ | 8.010e-008 | 8.010e-008 | -7.096 | -7.096 | 0.000 |
| | KHSO ₄ | 2.124e-008 | 2.124e-008 | -7.673 | -7.673 | 0.000 |
| | H ₂ SO ₄ | 8.115e-009 | 8.115e-009 | -8.091 | -8.091 | 0.000 |
| Zn | | 3.064e-007 | | | | |
| | Zn+2 | 2.260e-007 | 1.178e-007 | -6.646 | -6.929 | -0.283 |
| | ZnSO ₄ | 8.010e-008 | 8.010e-008 | -7.096 | -7.096 | 0.000 |
| | ZnCl+ | 2.159e-010 | 1.809e-010 | -9.666 | -9.743 | -0.077 |
| | ZnCl ₂ | 1.932e-013 | 1.932e-013 | -12.714 | -12.714 | 0.000 |
| | ZnOH+ | 3.004e-014 | 2.517e-014 | -13.522 | -13.599 | -0.077 |
| | Zn(OH)Cl | 6.029e-016 | 6.029e-016 | -15.220 | -15.220 | 0.000 |

| | | | | | |
|-----------|------------|------------|---------|---------|--------|
| ZnCl3- | 1.165e-016 | 9.758e-017 | -15.934 | -16.011 | -0.077 |
| ZnCl4-2 | 1.387e-018 | 6.763e-019 | -17.858 | -18.170 | -0.312 |
| Zn(OH)2 | 2.101e-020 | 2.101e-020 | -19.678 | -19.678 | 0.000 |
| Zn(OH)3- | 1.515e-029 | 1.269e-029 | -28.820 | -28.897 | -0.077 |
| Zn(OH)4-2 | 8.646e-040 | 4.216e-040 | -39.063 | -39.375 | -0.312 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -82.010 | -82.087 | -0.077 |

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

| Phase | SI | log IAP | log KT | |
|--------------------|---------|---------|--------|--------------------------|
| Al | -125.24 | 24.67 | 149.91 | Al |
| Al(g) | -175.95 | 24.67 | 200.62 | Al |
| Al2(SO4)3 | -34.02 | -15.12 | 18.90 | Al2(SO4)3 |
| Al2(SO4)3:6H2O | -16.68 | -15.12 | 1.56 | Al2(SO4)3:6H2O |
| Alum-K | -7.58 | -12.55 | -4.97 | KAl(SO4)2:12H2O |
| Alunite | -5.99 | -6.46 | -0.47 | KAl3(OH)6(SO4)2 |
| Anhydrite | -0.64 | -4.99 | -4.35 | CaSO4 |
| Antarcticite | -12.67 | -8.58 | 4.09 | CaCl2:6H2O |
| Antlerite | -20.40 | -11.67 | 8.73 | Cu3(SO4)(OH)4 |
| Aphthitalite | -14.96 | -18.85 | -3.89 | NaK3(SO4)2 |
| Arcanite | -8.14 | -9.98 | -1.84 | K2SO4 |
| Arsenolite | -31.36 | -51.20 | -19.84 | As2O3 |
| As | -46.66 | -3.97 | 42.68 | As |
| As2O5 | -21.11 | -18.97 | 2.14 | As2O5 |
| As4O6(cubi) | -62.57 | -102.40 | -39.82 | As4O6 |
| As4O6(mono) | -62.35 | -102.40 | -40.05 | As4O6 |
| Atacamite | -31.06 | -16.79 | 14.26 | Cu4Cl2(OH)6 |
| Bassanite | -1.28 | -4.99 | -3.71 | CaSO4:0.5H2O |
| Birnessite | -93.91 | -179.45 | -85.55 | Mn8O14:5H2O |
| Bischofite | -13.81 | -9.42 | 4.39 | MgCl2:6H2O |
| Bixbyite | -20.50 | -21.47 | -0.96 | Mn2O3 |
| Bloedite | -11.11 | -13.59 | -2.48 | Na2Mg(SO4)2:4H2O |
| Boehmite | -4.51 | 3.04 | 7.55 | AlO2H |
| Brochantite | -28.63 | -13.21 | 15.42 | Cu4(SO4)(OH)6 |
| Brucite | -15.04 | 1.24 | 16.28 | Mg(OH)2 |
| Ca | -123.33 | 16.50 | 139.83 | Ca |
| Ca(g) | -148.57 | 16.50 | 165.07 | Ca |
| Ca2Al2O5:8H2O | -49.32 | 10.25 | 59.57 | Ca2Al2O5:8H2O |
| Ca2Cl2(OH)2:H2O | -32.78 | -6.49 | 26.29 | Ca2Cl2(OH)2:H2O |
| Ca3(AsO4)2 | -30.52 | -12.72 | 17.80 | Ca3(AsO4)2 |
| Ca3Al2O6 | -100.69 | 12.34 | 113.03 | Ca3Al2O6 |
| Ca4Al2Fe2O10 | -122.66 | 17.82 | 140.48 | Ca4Al2Fe2O10 |
| Ca4Al2O7:13H2O | -92.84 | 14.42 | 107.25 | Ca4Al2O7:13H2O |
| Ca4Al2O7:19H2O | -89.27 | 14.42 | 103.68 | Ca4Al2O7:19H2O |
| Ca4Cl2(OH)6:13H2O | -70.66 | -2.33 | 68.33 | Ca4Cl2(OH)6:13H2O |
| CaAl2O4 | -38.74 | 8.17 | 46.91 | CaAl2O4 |
| CaAl2O4:10H2O | -29.83 | 8.17 | 37.99 | CaAl2O4:10H2O |
| CaAl4O7 | -54.33 | 14.26 | 68.59 | CaAl4O7 |
| Carnallite | -20.48 | -16.20 | 4.27 | KMgCl3:6H2O |
| CaSO4:0.5H2O(beta) | -1.45 | -4.99 | -3.54 | CaSO4:0.5H2O |
| Chalcanthite | -5.98 | -8.60 | -2.63 | CuSO4:5H2O |
| Chalcocyanite | -11.52 | -8.60 | 2.91 | CuSO4 |
| Chloromagnesite | -31.23 | -9.42 | 21.82 | MgCl2 |
| Cl2(g) | -28.07 | -25.08 | 2.99 | Cl2 |
| Claudetite | -31.40 | -51.20 | -19.80 | As2O3 |
| Corundum | -12.20 | 6.09 | 18.29 | Al2O3 |
| Cu | -18.61 | 12.88 | 31.50 | Cu |
| Cu(g) | -70.77 | 12.88 | 83.66 | Cu |
| CuCl2 | -15.91 | -12.19 | 3.72 | CuCl2 |
| Cuprite | -24.26 | -26.17 | -1.91 | Cu2O |
| Delafossite | -4.95 | -11.38 | -6.44 | CuFeO2 |
| Diaspore | -4.10 | 3.04 | 7.15 | AlHO2 |
| Epsomite | -3.87 | -5.83 | -1.96 | MgSO4:7H2O |
| Ettringite | -65.09 | -2.63 | 62.46 | Ca6Al2(SO4)3(OH)12:26H2O |
| Fe | -44.17 | 14.85 | 59.02 | Fe |
| Fe(OH)2 | -13.46 | 0.43 | 13.89 | Fe(OH)2 |

| | | | | |
|-------------------------|---------|--------|--------|-------------------------|
| Fe(OH)3 | -3.94 | 1.70 | 5.64 | Fe(OH)3 |
| Fe2(SO4)3 | -20.85 | -17.80 | 3.05 | Fe2(SO4)3 |
| FeO | -13.09 | 0.43 | 13.52 | FeO |
| Ferrite-Ca | -16.01 | 5.49 | 21.50 | CaFe2O4 |
| Ferrite-Cu | -8.41 | 1.87 | 10.28 | CuFe2O4 |
| Ferrite-Dicalcium | -49.23 | 7.57 | 56.80 | Ca2Fe2O5 |
| Ferrite-Mg | -16.38 | 4.64 | 21.02 | MgFe2O4 |
| Ferrite-Zn | -10.64 | 1.06 | 11.70 | ZnFe2O4 |
| FeSO4 | -9.25 | -6.64 | 2.61 | FeSO4 |
| Gibbsite | -4.70 | 3.04 | 7.74 | Al(OH)3 |
| Glauberite | -7.27 | -12.74 | -5.47 | Na2Ca(SO4)2 |
| Goethite | 1.17 | 1.70 | 0.53 | FeOOH |
| Gypsum | -0.46 | -4.99 | -4.53 | CaSO4:2H2O |
| H2(g) | -28.58 | -31.68 | -3.10 | H2 |
| H2O(g) | -1.59 | -0.00 | 1.59 | H2O |
| Halite | -7.23 | -5.67 | 1.56 | NaCl |
| Hausmannite | -31.06 | -20.91 | 10.14 | Mn3O4 |
| HCl(g) | -11.63 | -5.33 | 6.30 | HCl |
| Hematite | 3.33 | 3.40 | 0.08 | Fe2O3 |
| Hercynite | -22.28 | 6.52 | 28.80 | FeAl2O4 |
| Hexahydrite | -4.11 | -5.83 | -1.73 | MgSO4:6H2O |
| Hydrophilite | -20.32 | -8.57 | 11.75 | CaCl2 |
| Ice | -0.14 | -0.00 | 0.14 | H2O |
| Jarosite | -1.08 | -10.49 | -9.41 | KFe3(SO4)2(OH)6 |
| Jarosite-Na | -3.93 | -9.38 | -5.45 | NaFe3(SO4)2(OH)6 |
| K | -65.22 | 5.75 | 70.98 | K |
| K(g) | -75.83 | 5.75 | 81.58 | K |
| K2O | -86.95 | -2.91 | 84.04 | K2O |
| K3H(SO4)2 | -14.88 | -18.51 | -3.62 | K3H(SO4)2 |
| Kainite | -12.30 | -12.62 | -0.31 | KMgClSO4:3H2O |
| KAl(SO4)2 | -15.82 | -12.55 | 3.27 | KAl(SO4)2 |
| Katoite | -66.61 | 12.34 | 78.94 | Ca3Al2H12O12 |
| Kieserite | -5.56 | -5.83 | -0.27 | MgSO4:H2O |
| KMgCl3 | -37.45 | -16.20 | 21.25 | KMgCl3 |
| KMgCl3:2H2O | -30.17 | -16.20 | 13.96 | KMgCl3:2H2O |
| Lammerite | -25.13 | -23.57 | 1.55 | Cu3(AsO4)2 |
| Lawrencite | -19.28 | -10.23 | 9.05 | FeCl2 |
| Leonite | -11.70 | -15.81 | -4.11 | K2Mg(SO4)2:4H2O |
| Lime | -30.49 | 2.08 | 32.57 | CaO |
| Magnetite | -6.58 | 3.84 | 10.42 | Fe3O4 |
| Manganite | -10.57 | -10.73 | -0.16 | MnO(OH) |
| Manganosite | -17.36 | 0.55 | 17.92 | MnO |
| Mayenite | -426.54 | 67.61 | 494.15 | Ca12Al14O33 |
| Melanterite | -4.24 | -6.64 | -2.40 | FeSO4:7H2O |
| Mercallite | -7.09 | -8.53 | -1.44 | KHSO4 |
| Mg | -106.86 | 15.66 | 122.52 | Mg |
| Mg(g) | -126.59 | 15.66 | 142.25 | Mg |
| Mg1.25SO4(OH)0.5:0.5H2O | -10.72 | -5.52 | 5.20 | Mg1.25SO4(OH)0.5:0.5H2O |
| Mg1.5SO4(OH) | -14.42 | -5.21 | 9.21 | Mg1.5SO4(OH) |
| MgCl2:2H2O | -22.15 | -9.42 | 12.73 | MgCl2:2H2O |
| MgCl2:4H2O | -16.72 | -9.42 | 7.30 | MgCl2:4H2O |
| MgCl2:H2O | -25.49 | -9.42 | 16.07 | MgCl2:H2O |
| MgOHCl | -19.98 | -4.09 | 15.89 | MgOHCl |
| MgSO4 | -10.66 | -5.83 | 4.83 | MgSO4 |
| Mirabilite | -6.60 | -7.76 | -1.15 | Na2SO4:10H2O |
| Misenite | -50.06 | -61.13 | -11.08 | K8H6(SO4)7 |
| Mn | -67.96 | 14.97 | 82.93 | Mn |
| Mn(OH)2(am) | -14.76 | 0.55 | 15.31 | Mn(OH)2 |
| Mn(OH)3 | -17.07 | -10.73 | 6.34 | Mn(OH)3 |
| MnCl2:2H2O | -14.10 | -10.11 | 4.00 | MnCl2:2H2O |
| MnCl2:4H2O | -12.86 | -10.11 | 2.75 | MnCl2:4H2O |
| MnCl2:H2O | -15.65 | -10.11 | 5.54 | MnCl2:H2O |
| MnO2(gamma) | -13.97 | -30.09 | -16.13 | MnO2 |
| MnSO4 | -9.13 | -6.52 | 2.61 | MnSO4 |
| Molysite | -27.75 | -14.28 | 13.47 | FeCl3 |
| Na | -60.50 | 6.87 | 67.37 | Na |
| Na(g) | -73.99 | 6.87 | 80.86 | Na |

| | | | | |
|------------------|---------|---------|--------|--------------------|
| Na2O | -68.10 | -0.68 | 67.42 | Na2O |
| Na3H(SO4)2 | -14.28 | -15.17 | -0.89 | Na3H(SO4)2 |
| Na4Ca(SO4)3:2H2O | -14.60 | -20.50 | -5.89 | Na4Ca(SO4)3:2H2O |
| NaFeO2 | -18.52 | 1.36 | 19.88 | NaFeO2 |
| Nantokite | -11.65 | -18.41 | -6.77 | CuCl |
| O2(g) | -25.94 | -28.84 | -2.89 | O2 |
| Oxychloride-Mg | -28.68 | -2.85 | 25.83 | Mg2Cl(OH)3:4H2O |
| Pentahydrate | -4.44 | -5.83 | -1.39 | MgSO4:5H2O |
| Periclase | -20.09 | 1.24 | 21.33 | MgO |
| Picromerite | -11.37 | -15.81 | -4.44 | K2Mg(SO4)2:6H2O |
| Polyhalite | -11.47 | -25.79 | -14.31 | K2MgCa2(SO4)4:2H2O |
| Portlandite | -20.46 | 2.08 | 22.55 | Ca(OH)2 |
| Pyrolusite | -12.43 | -30.09 | -17.66 | MnO2 |
| Scacchite | -18.85 | -10.11 | 8.74 | MnCl2 |
| Spinel | -30.28 | 7.33 | 37.61 | Al2MgO4 |
| Starkeyite | -4.83 | -5.83 | -1.00 | MgSO4:4H2O |
| Sylvite | -7.61 | -6.78 | 0.83 | KCl |
| Syngenite | -7.37 | -14.97 | -7.60 | K2Ca(SO4)2:H2O |
| Tachyhydrite | -44.56 | -27.41 | 17.14 | Mg2CaCl6:12H2O |
| Tenorite | -9.18 | -1.53 | 7.65 | CuO |
| Thenardite | -7.40 | -7.75 | -0.36 | Na2SO4 |
| Todorokite | -79.31 | -125.13 | -45.82 | Mn7O12:3H2O |
| Wustite | -11.86 | 0.54 | 12.40 | Fe.9470 |
| Zincite | -13.55 | -2.35 | 11.20 | ZnO |
| Zn | -56.72 | 12.07 | 68.79 | Zn |
| Zn(ClO4)2:6H2O | -165.43 | -159.80 | 5.63 | Zn(ClO4)2:6H2O |
| Zn(g) | -73.34 | 12.07 | 85.41 | Zn |
| Zn(OH)2(beta) | -14.28 | -2.35 | 11.93 | Zn(OH)2 |
| Zn(OH)2(epsilon) | -14.01 | -2.35 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -14.23 | -2.35 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -25.32 | -10.03 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -19.35 | -11.77 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -35.33 | -26.02 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -40.28 | -21.19 | 19.09 | Zn3O(SO4)2 |
| ZnCl2 | -20.09 | -13.01 | 7.08 | ZnCl2 |
| ZnSO4 | -12.95 | -9.42 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -7.72 | -9.42 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -7.54 | -9.42 | -1.88 | ZnSO4:7H2O |
| ZnSO4:H2O | -8.87 | -9.42 | -0.55 | ZnSO4:H2O |

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 1.

Mixture 1.

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

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

| Elements | Molality | Moles |
|----------|------------|------------|
| Al | 1.071e-003 | 4.284e-003 |
| As | 5.780e-006 | 2.312e-005 |
| Ca | 6.207e-003 | 2.483e-002 |
| Cl | 1.156e-003 | 4.624e-003 |
| Cu | 8.543e-005 | 3.417e-004 |
| Fe | 7.619e-004 | 3.048e-003 |
| K | 3.606e-004 | 1.442e-003 |
| Mg | 1.006e-003 | 4.022e-003 |
| Mn | 2.553e-004 | 1.021e-003 |
| Na | 2.345e-003 | 9.379e-003 |

| | | |
|----|------------|------------|
| S | 1.087e-002 | 4.348e-002 |
| Zn | 2.013e-005 | 8.054e-005 |

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

| | | | |
|--|---|---------------|-------------------------------|
| pH | = | 2.417 | Charge balance |
| pe | = | 13.218 | Adjusted to redox equilibrium |
| Activity of water | = | 1.000 | |
| Ionic strength | = | 3.453e-002 | |
| Mass of water (kg) | = | 4.000e+000 | |
| Total alkalinity (eq/kg) | = | -6.885e-003 | |
| Total carbon (mol/kg) | = | 0.000e+000 | |
| Total CO2 (mol/kg) | = | 0.000e+000 | |
| Temperature (deg C) | = | 25.000 | |
| Electrical balance (eq) | = | 2.376e-002 | |
| Percent error, 100*(Cat- An)/(Cat+ An) | = | 15.37 | |
| Iterations | = | 7 | |
| Total H | = | 4.442301e+002 | |
| Total O | = | 2.222778e+002 | |

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|----------------|------------|------------|--------------|--------------|-----------|
| H+ | 4.397e-003 | 3.831e-003 | -2.357 | -2.417 | -0.060 |
| OH- | 3.001e-012 | 2.514e-012 | -11.523 | -11.600 | -0.077 |
| H2O | 5.553e+001 | 9.996e-001 | 1.744 | -0.000 | 0.000 |
| Al | 1.071e-003 | | | | |
| AlSO4+ | 5.017e-004 | 4.222e-004 | -3.300 | -3.375 | -0.075 |
| Al+3 | 4.384e-004 | 1.234e-004 | -3.358 | -3.909 | -0.550 |
| Al(SO4)2- | 1.302e-004 | 1.095e-004 | -3.885 | -3.960 | -0.075 |
| AlOH+2 | 7.145e-007 | 3.608e-007 | -6.146 | -6.443 | -0.297 |
| Al2(OH)2+4 | 2.900e-010 | 2.117e-011 | -9.538 | -10.674 | -1.137 |
| Al(OH)2+ | 2.598e-010 | 2.186e-010 | -9.585 | -9.660 | -0.075 |
| HA1O2 | 8.306e-014 | 8.306e-014 | -13.081 | -13.081 | 0.000 |
| Al3(OH)4+5 | 6.268e-015 | 1.149e-016 | -14.203 | -15.940 | -1.737 |
| AlO2- | 8.827e-018 | 7.428e-018 | -17.054 | -17.129 | -0.075 |
| NaAlO2 | 2.735e-021 | 2.735e-021 | -20.563 | -20.563 | 0.000 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -68.805 | -72.211 | -3.406 |
| As(-3) | 0.000e+000 | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -116.212 | -116.212 | 0.000 |
| As(3) | 6.546e-018 | | | | |
| HAsO2 | 3.493e-018 | 3.493e-018 | -17.457 | -17.457 | 0.000 |
| As(OH)3 | 3.053e-018 | 3.053e-018 | -17.515 | -17.515 | 0.000 |
| H2AsO3- | 5.792e-025 | 4.874e-025 | -24.237 | -24.312 | -0.075 |
| AsO2- | 5.539e-025 | 4.661e-025 | -24.257 | -24.331 | -0.075 |
| AsO2OH-2 | 2.503e-033 | 1.243e-033 | -32.601 | -32.906 | -0.304 |
| HAsS2 | 0.000e+000 | 0.000e+000 | -193.605 | -193.605 | 0.000 |
| As(5) | 5.780e-006 | | | | |
| H2AsO4- | 3.686e-006 | 3.102e-006 | -5.433 | -5.508 | -0.075 |
| H3AsO4 | 2.093e-006 | 2.093e-006 | -5.679 | -5.679 | 0.000 |
| HAsO4-2 | 2.707e-010 | 1.344e-010 | -9.567 | -9.872 | -0.304 |
| AsO4-3 | 4.368e-019 | 9.003e-020 | -18.360 | -19.046 | -0.686 |
| Ca | 6.207e-003 | | | | |
| Ca+2 | 4.932e-003 | 2.608e-003 | -2.307 | -2.584 | -0.277 |
| CaSO4 | 1.273e-003 | 1.273e-003 | -2.895 | -2.895 | 0.000 |
| CaCl+ | 6.319e-007 | 5.317e-007 | -6.199 | -6.274 | -0.075 |
| CaCl2 | 6.016e-010 | 6.016e-010 | -9.221 | -9.221 | 0.000 |
| CaOH+ | 1.142e-013 | 9.613e-014 | -12.942 | -13.017 | -0.075 |
| Cl(-1) | 1.156e-003 | | | | |
| Cl- | 1.154e-003 | 9.619e-004 | -2.938 | -3.017 | -0.079 |
| HCl | 8.276e-007 | 8.276e-007 | -6.082 | -6.082 | 0.000 |
| CaCl+ | 6.319e-007 | 5.317e-007 | -6.199 | -6.274 | -0.075 |
| MgCl+ | 3.339e-007 | 2.810e-007 | -6.476 | -6.551 | -0.075 |
| NaCl | 3.263e-007 | 3.263e-007 | -6.486 | -6.486 | 0.000 |
| MnCl+ | 2.286e-007 | 1.923e-007 | -6.641 | -6.716 | -0.075 |

| | | | | | |
|------------|------------|------------|---------|---------|--------|
| CuCl+ | 1.004e-007 | 8.450e-008 | -6.998 | -7.073 | -0.075 |
| FeCl+ | 4.368e-008 | 3.675e-008 | -7.360 | -7.435 | -0.075 |
| FeCl+2 | 2.636e-008 | 1.331e-008 | -7.579 | -7.876 | -0.297 |
| ZnCl+ | 1.490e-008 | 1.254e-008 | -7.827 | -7.902 | -0.075 |
| FeCl2+ | 1.232e-008 | 1.037e-008 | -7.909 | -7.984 | -0.075 |
| KCl | 9.458e-009 | 9.458e-009 | -8.024 | -8.024 | 0.000 |
| CaCl2 | 6.016e-010 | 6.016e-010 | -9.221 | -9.221 | 0.000 |
| CuCl2 | 4.281e-011 | 4.281e-011 | -10.368 | -10.368 | 0.000 |
| ZnCl2 | 1.409e-011 | 1.409e-011 | -10.851 | -10.851 | 0.000 |
| FeCl2 | 1.897e-013 | 1.897e-013 | -12.722 | -12.722 | 0.000 |
| Zn(OH)Cl | 5.594e-014 | 5.594e-014 | -13.252 | -13.252 | 0.000 |
| MnCl3- | 4.620e-014 | 3.888e-014 | -13.335 | -13.410 | -0.075 |
| ZnCl3- | 8.893e-015 | 7.483e-015 | -14.051 | -14.126 | -0.075 |
| ZnCl4-2 | 1.099e-016 | 5.456e-017 | -15.959 | -16.263 | -0.304 |
| CuCl2- | 7.754e-017 | 6.525e-017 | -16.110 | -16.185 | -0.075 |
| FeCl4- | 1.370e-017 | 1.153e-017 | -16.863 | -16.938 | -0.075 |
| FeCl4-2 | 1.022e-018 | 5.072e-019 | -17.991 | -18.295 | -0.304 |
| CuCl3-2 | 8.118e-019 | 4.031e-019 | -18.091 | -18.395 | -0.304 |
| CuCl4-2 | 1.497e-021 | 7.433e-022 | -20.825 | -21.129 | -0.304 |
| Cl(1) | 1.978e-025 | | | | |
| HClO | 1.978e-025 | 1.978e-025 | -24.704 | -24.704 | 0.000 |
| ClO- | 1.655e-030 | 1.393e-030 | -29.781 | -29.856 | -0.075 |
| Cl(3) | 0.000e+000 | | | | |
| HClO2 | 0.000e+000 | 0.000e+000 | -48.837 | -48.837 | 0.000 |
| ClO2- | 0.000e+000 | 0.000e+000 | -49.515 | -49.590 | -0.075 |
| Cl(5) | 0.000e+000 | | | | |
| ClO3- | 0.000e+000 | 0.000e+000 | -55.395 | -55.472 | -0.077 |
| Cl(7) | 0.000e+000 | | | | |
| ClO4- | 0.000e+000 | 0.000e+000 | -65.578 | -65.655 | -0.077 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -69.414 | -69.489 | -0.075 |
| Cu(1) | 1.343e-015 | | | | |
| Cu+ | 1.265e-015 | 1.064e-015 | -14.898 | -14.973 | -0.075 |
| CuCl2- | 7.754e-017 | 6.525e-017 | -16.110 | -16.185 | -0.075 |
| CuCl3-2 | 8.118e-019 | 4.031e-019 | -18.091 | -18.395 | -0.304 |
| Cu(2) | 8.543e-005 | | | | |
| Cu+2 | 6.074e-005 | 3.212e-005 | -4.217 | -4.493 | -0.277 |
| CuSO4 | 2.459e-005 | 2.459e-005 | -4.609 | -4.609 | 0.000 |
| CuCl+ | 1.004e-007 | 8.450e-008 | -6.998 | -7.073 | -0.075 |
| CuOH+ | 5.137e-010 | 4.323e-010 | -9.289 | -9.364 | -0.075 |
| CuCl2 | 4.281e-011 | 4.281e-011 | -10.368 | -10.368 | 0.000 |
| CuCl4-2 | 1.497e-021 | 7.433e-022 | -20.825 | -21.129 | -0.304 |
| CuO2-2 | 1.066e-034 | 5.292e-035 | -33.972 | -34.276 | -0.304 |
| Fe(2) | 1.270e-004 | | | | |
| Fe+2 | 9.919e-005 | 5.245e-005 | -4.004 | -4.280 | -0.277 |
| FeSO4 | 2.778e-005 | 2.778e-005 | -4.556 | -4.556 | 0.000 |
| FeCl+ | 4.368e-008 | 3.675e-008 | -7.360 | -7.435 | -0.075 |
| FeOH+ | 5.143e-012 | 4.328e-012 | -11.289 | -11.364 | -0.075 |
| FeCl2 | 1.897e-013 | 1.897e-013 | -12.722 | -12.722 | 0.000 |
| FeCl4-2 | 1.022e-018 | 5.072e-019 | -17.991 | -18.295 | -0.304 |
| Fe(OH)2 | 8.971e-021 | 8.971e-021 | -20.047 | -20.047 | 0.000 |
| Fe(OH)3- | 1.107e-028 | 9.319e-029 | -27.956 | -28.031 | -0.075 |
| Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -40.310 | -40.614 | -0.304 |
| Fe(3) | 6.349e-004 | | | | |
| Fe+3 | 2.950e-004 | 8.306e-005 | -3.530 | -4.081 | -0.550 |
| FeOH+2 | 2.771e-004 | 1.399e-004 | -3.557 | -3.854 | -0.297 |
| FeSO4+ | 3.192e-005 | 2.686e-005 | -4.496 | -4.571 | -0.075 |
| Fe(OH)2+ | 1.437e-005 | 1.209e-005 | -4.843 | -4.918 | -0.075 |
| Fe2(OH)2+4 | 7.219e-006 | 5.271e-007 | -5.142 | -6.278 | -1.137 |
| Fe(SO4)2- | 1.804e-006 | 1.518e-006 | -5.744 | -5.819 | -0.075 |
| Fe3(OH)4+5 | 7.267e-008 | 1.332e-009 | -7.139 | -8.876 | -1.737 |
| FeCl+2 | 2.636e-008 | 1.331e-008 | -7.579 | -7.876 | -0.297 |
| FeCl2+ | 1.232e-008 | 1.037e-008 | -7.909 | -7.984 | -0.075 |
| Fe(OH)3 | 1.476e-009 | 1.476e-009 | -8.831 | -8.831 | 0.000 |
| Fe(OH)4- | 1.150e-016 | 9.673e-017 | -15.939 | -16.014 | -0.075 |
| FeCl4- | 1.370e-017 | 1.153e-017 | -16.863 | -16.938 | -0.075 |
| H(0) | 8.464e-035 | | | | |
| H2 | 4.232e-035 | 4.268e-035 | -34.373 | -34.370 | 0.004 |

| | | | | | | |
|------------|------------|------------|----------|----------|--------|--|
| K | 3.606e-004 | | | | | |
| K+ | 3.511e-004 | 2.928e-004 | -3.455 | -3.533 | -0.079 | |
| KSO4- | 9.388e-006 | 7.900e-006 | -5.027 | -5.102 | -0.075 | |
| KHSO4 | 2.670e-008 | 2.670e-008 | -7.574 | -7.574 | 0.000 | |
| KCl | 9.458e-009 | 9.458e-009 | -8.024 | -8.024 | 0.000 | |
| KOH | 2.649e-016 | 2.649e-016 | -15.577 | -15.577 | 0.000 | |
| Mg | 1.006e-003 | | | | | |
| Mg+2 | 6.713e-004 | 3.741e-004 | -3.173 | -3.427 | -0.254 | |
| MgSO4 | 3.339e-004 | 3.339e-004 | -3.476 | -3.476 | 0.000 | |
| MgCl+ | 3.339e-007 | 2.810e-007 | -6.476 | -6.551 | -0.075 | |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -42.655 | -43.792 | -1.137 | |
| Mn(2) | 2.553e-004 | | | | | |
| Mn+2 | 1.776e-004 | 9.391e-005 | -3.751 | -4.027 | -0.277 | |
| MnSO4 | 7.744e-005 | 7.744e-005 | -4.111 | -4.111 | 0.000 | |
| MnCl+ | 2.286e-007 | 1.923e-007 | -6.641 | -6.716 | -0.075 | |
| MnOH+ | 7.485e-013 | 6.299e-013 | -12.126 | -12.201 | -0.075 | |
| MnCl3- | 4.620e-014 | 3.888e-014 | -13.335 | -13.410 | -0.075 | |
| Mn2OH+3 | 2.855e-016 | 6.338e-017 | -15.544 | -16.198 | -0.654 | |
| Mn(OH)2 | 4.034e-022 | 4.034e-022 | -21.394 | -21.394 | 0.000 | |
| Mn2(OH)3+ | 2.344e-025 | 1.973e-025 | -24.630 | -24.705 | -0.075 | |
| Mn(OH)3- | 1.173e-031 | 9.875e-032 | -30.931 | -31.005 | -0.075 | |
| Mn(OH)4-2 | 0.000e+000 | 0.000e+000 | -42.357 | -42.661 | -0.304 | |
| Mn(3) | 1.864e-016 | | | | | |
| Mn+3 | 1.864e-016 | 4.137e-017 | -15.730 | -16.383 | -0.654 | |
| Mn(6) | 0.000e+000 | | | | | |
| MnO4-2 | 0.000e+000 | 0.000e+000 | -49.965 | -50.269 | -0.304 | |
| Mn(7) | 0.000e+000 | | | | | |
| MnO4- | 0.000e+000 | 0.000e+000 | -46.331 | -46.408 | -0.077 | |
| Na | 2.345e-003 | | | | | |
| Na+ | 2.294e-003 | 1.930e-003 | -2.639 | -2.714 | -0.075 | |
| NaSO4- | 5.065e-005 | 4.263e-005 | -4.295 | -4.370 | -0.075 | |
| NaCl | 3.263e-007 | 3.263e-007 | -6.486 | -6.486 | 0.000 | |
| NaOH | 8.372e-016 | 8.372e-016 | -15.077 | -15.077 | 0.000 | |
| NaAlO2 | 2.735e-021 | 2.735e-021 | -20.563 | -20.563 | 0.000 | |
| O(0) | 6.929e-024 | | | | | |
| O2 | 3.464e-024 | 3.493e-024 | -23.460 | -23.457 | 0.004 | |
| S(-2) | 0.000e+000 | | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -91.669 | -91.669 | 0.000 | |
| HS- | 0.000e+000 | 0.000e+000 | -96.185 | -96.262 | -0.077 | |
| S-2 | 0.000e+000 | 0.000e+000 | -106.481 | -106.771 | -0.290 | |
| S2-2 | 0.000e+000 | 0.000e+000 | -170.690 | -170.994 | -0.304 | |
| HAsS2 | 0.000e+000 | 0.000e+000 | -193.605 | -193.605 | 0.000 | |
| S3-2 | 0.000e+000 | 0.000e+000 | -234.954 | -235.259 | -0.304 | |
| S4-2 | 0.000e+000 | 0.000e+000 | -299.446 | -299.750 | -0.304 | |
| S5-2 | 0.000e+000 | 0.000e+000 | -364.154 | -364.458 | -0.304 | |
| S(2) | 0.000e+000 | | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -96.041 | -96.345 | -0.304 | |
| HS2O3- | 0.000e+000 | 0.000e+000 | -97.673 | -97.748 | -0.075 | |
| S(3) | 0.000e+000 | | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -92.712 | -93.002 | -0.290 | |
| S(4) | 5.199e-033 | | | | | |
| HSO3- | 3.345e-033 | 2.815e-033 | -32.476 | -32.551 | -0.075 | |
| H2SO3 | 1.034e-033 | 1.034e-033 | -32.986 | -32.986 | 0.000 | |
| SO2 | 8.208e-034 | 8.208e-034 | -33.086 | -33.086 | 0.000 | |
| SO3-2 | 8.537e-038 | 4.311e-038 | -37.069 | -37.365 | -0.297 | |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -49.121 | -49.425 | -0.304 | |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -115.869 | -116.173 | -0.304 | |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -166.710 | -167.014 | -0.304 | |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -246.431 | -246.735 | -0.304 | |
| S(5) | 0.000e+000 | | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -69.627 | -69.931 | -0.304 | |
| S(6) | 1.087e-002 | | | | | |
| SO4-2 | 6.731e-003 | 3.342e-003 | -2.172 | -2.476 | -0.304 | |
| HSO4- | 1.537e-003 | 1.293e-003 | -2.813 | -2.888 | -0.075 | |
| CaSO4 | 1.273e-003 | 1.273e-003 | -2.895 | -2.895 | 0.000 | |
| AlSO4+ | 5.017e-004 | 4.222e-004 | -3.300 | -3.375 | -0.075 | |
| MgSO4 | 3.339e-004 | 3.339e-004 | -3.476 | -3.476 | 0.000 | |

| | | | | | |
|-----------|------------|------------|---------|---------|--------|
| Al(SO4)2- | 1.302e-004 | 1.095e-004 | -3.885 | -3.960 | -0.075 |
| MnSO4 | 7.744e-005 | 7.744e-005 | -4.111 | -4.111 | 0.000 |
| NaSO4- | 5.065e-005 | 4.263e-005 | -4.295 | -4.370 | -0.075 |
| FeSO4+ | 3.192e-005 | 2.686e-005 | -4.496 | -4.571 | -0.075 |
| FeSO4 | 2.778e-005 | 2.778e-005 | -4.556 | -4.556 | 0.000 |
| CuSO4 | 2.459e-005 | 2.459e-005 | -4.609 | -4.609 | 0.000 |
| KSO4- | 9.388e-006 | 7.900e-006 | -5.027 | -5.102 | -0.075 |
| ZnSO4 | 5.448e-006 | 5.448e-006 | -5.264 | -5.264 | 0.000 |
| Fe(SO4)2- | 1.804e-006 | 1.518e-006 | -5.744 | -5.819 | -0.075 |
| KHSO4 | 2.670e-008 | 2.670e-008 | -7.574 | -7.574 | 0.000 |
| H2SO4 | 4.674e-009 | 4.674e-009 | -8.330 | -8.330 | 0.000 |
| S(7) | 0.000e+000 | | | | |
| S2O8-2 | 0.000e+000 | 0.000e+000 | -43.665 | -43.969 | -0.304 |
| S(8) | 1.560e-034 | | | | |
| HSO5- | 1.560e-034 | 1.313e-034 | -33.807 | -33.882 | -0.075 |
| Zn | 2.013e-005 | | | | |
| Zn+2 | 1.467e-005 | 7.758e-006 | -4.834 | -5.110 | -0.277 |
| ZnSO4 | 5.448e-006 | 5.448e-006 | -5.264 | -5.264 | 0.000 |
| ZnCl+ | 1.490e-008 | 1.254e-008 | -7.827 | -7.902 | -0.075 |
| ZnCl2 | 1.409e-011 | 1.409e-011 | -10.851 | -10.851 | 0.000 |
| ZnOH+ | 2.638e-012 | 2.220e-012 | -11.579 | -11.654 | -0.075 |
| Zn(OH)Cl | 5.594e-014 | 5.594e-014 | -13.252 | -13.252 | 0.000 |
| ZnCl3- | 8.893e-015 | 7.483e-015 | -14.051 | -14.126 | -0.075 |
| ZnCl4-2 | 1.099e-016 | 5.456e-017 | -15.959 | -16.263 | -0.304 |
| Zn(OH)2 | 2.481e-018 | 2.481e-018 | -17.605 | -17.605 | 0.000 |
| Zn(OH)3- | 2.385e-027 | 2.007e-027 | -26.623 | -26.698 | -0.075 |
| Zn(OH)4-2 | 1.798e-037 | 8.927e-038 | -36.745 | -37.049 | -0.304 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -69.414 | -69.489 | -0.075 |

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

| Phase | SI | log IAP | log KT | |
|-----------------|---------|---------|---------|------------------|
| Al | -128.98 | 20.93 | 149.91 | Al |
| Al(g) | -179.68 | 20.93 | 200.62 | Al |
| Al2(SO4)3 | -34.14 | -15.24 | 18.90 | Al2(SO4)3 |
| Al2(SO4)3:6H2O | -16.80 | -15.25 | 1.56 | Al2(SO4)3:6H2O |
| Alabandite | -97.45 | -97.87 | -0.42 | MnS |
| Alum-K | -7.43 | -12.40 | -4.97 | KAl(SO4)2:12H2O |
| Alunite | -5.24 | -5.71 | -0.47 | KAl3(OH)6(SO4)2 |
| Anhydrite | -0.71 | -5.06 | -4.35 | CaSO4 |
| Antarcticite | -12.71 | -8.62 | 4.09 | CaCl2:6H2O |
| Antlerite | -15.02 | -6.29 | 8.73 | Cu3(SO4)(OH)4 |
| Aphthitalite | -14.38 | -18.27 | -3.89 | NaK3(SO4)2 |
| Arcanite | -7.70 | -9.54 | -1.84 | K2SO4 |
| Arsenolite | -33.61 | -53.46 | -19.84 | As2O3 |
| Arsenopyrite | -155.15 | -169.60 | -14.45 | FeAsS |
| As | -51.82 | -9.14 | 42.68 | As |
| As2O5 | -17.99 | -15.85 | 2.14 | As2O5 |
| As4O6(cubi) | -67.09 | -106.91 | -39.82 | As4O6 |
| As4O6(mono) | -66.86 | -106.91 | -40.05 | As4O6 |
| Atacamite | -23.77 | -9.51 | 14.26 | Cu4Cl2(OH)6 |
| Bassanite | -1.35 | -5.06 | -3.71 | CaSO4:0.5H2O |
| Birnessite | -75.73 | -161.28 | -85.55 | Mn8O14:5H2O |
| Bischofite | -13.85 | -9.46 | 4.39 | MgCl2:6H2O |
| Bixbyite | -17.30 | -18.27 | -0.96 | Mn2O3 |
| Bloedite | -11.33 | -13.81 | -2.48 | Na2Mg(SO4)2:4H2O |
| Boehmite | -4.21 | 3.34 | 7.55 | AlO2H |
| Bornite | -341.51 | -444.05 | -102.53 | Cu5FeS4 |
| Brochantite | -21.37 | -5.95 | 15.42 | Cu4(SO4)(OH)6 |
| Brucite | -14.88 | 1.41 | 16.28 | Mg(OH)2 |
| Ca | -125.85 | 13.98 | 139.83 | Ca |
| Ca(g) | -151.09 | 13.98 | 165.07 | Ca |
| Ca2Al2O5:8H2O | -48.39 | 11.18 | 59.57 | Ca2Al2O5:8H2O |
| Ca2Cl2(OH)2:H2O | -32.66 | -6.37 | 26.29 | Ca2Cl2(OH)2:H2O |
| Ca3(AsO4)2 | -26.90 | -9.10 | 17.80 | Ca3(AsO4)2 |
| Ca3Al2O6 | -99.60 | 13.43 | 113.03 | Ca3Al2O6 |

| | | | | |
|--------------------|---------|---------|--------|--------------------------|
| Ca4Al2Fe2O10 | -118.46 | 22.02 | 140.48 | Ca4Al2Fe2O10 |
| Ca4Al2O7:13H2O | -91.58 | 15.68 | 107.25 | Ca4Al2O7:13H2O |
| Ca4Al2O7:19H2O | -88.00 | 15.68 | 103.68 | Ca4Al2O7:19H2O |
| Ca4Cl2(OH)6:13H2O | -70.20 | -1.87 | 68.33 | Ca4Cl2(OH)6:13H2O |
| CaAl2O4 | -37.98 | 8.93 | 46.91 | CaAl2O4 |
| CaAl2O4:10H2O | -29.06 | 8.93 | 37.99 | CaAl2O4:10H2O |
| CaAl4O7 | -52.98 | 15.62 | 68.59 | CaAl4O7 |
| Carnallite | -20.28 | -16.01 | 4.27 | KMgCl3:6H2O |
| CaSO4:0.5H2O(beta) | -1.52 | -5.06 | -3.54 | CaSO4:0.5H2O |
| Chalcanthite | -4.34 | -6.97 | -2.63 | CuSO4:5H2O |
| Chalcocite | -89.05 | -123.79 | -34.74 | Cu2S |
| Chalcocyanite | -9.88 | -6.97 | 2.91 | CuSO4 |
| Chalcopyrite | -163.86 | -196.46 | -32.60 | CuFeS2 |
| Chloromagnesite | -31.28 | -9.46 | 21.82 | MgCl2 |
| Cl2(g) | -25.59 | -22.60 | 2.99 | Cl2 |
| Claudetite | -33.66 | -53.46 | -19.80 | As2O3 |
| Corundum | -11.61 | 6.68 | 18.29 | Al2O3 |
| Covellite | -75.48 | -98.34 | -22.86 | CuS |
| Cu | -19.43 | 12.07 | 31.50 | Cu |
| Cu(g) | -71.59 | 12.07 | 83.66 | Cu |
| CuCl2 | -14.25 | -10.53 | 3.72 | CuCl2 |
| Cuprite | -23.21 | -25.11 | -1.91 | Cu2O |
| Delafossite | -2.95 | -9.39 | -6.44 | CuFeO2 |
| Diaspore | -3.81 | 3.34 | 7.15 | AlHO2 |
| Epsomite | -3.94 | -5.90 | -1.96 | MgSO4:7H2O |
| Ettringite | -64.22 | -1.75 | 62.46 | Ca6Al2(SO4)3(OH)12:26H2O |
| Fe | -46.74 | 12.28 | 59.02 | Fe |
| Fe(OH)2 | -13.34 | 0.55 | 13.89 | Fe(OH)2 |
| Fe(OH)3 | -2.47 | 3.17 | 5.64 | Fe(OH)3 |
| Fe2(SO4)3 | -18.64 | -15.59 | 3.05 | Fe2(SO4)3 |
| FeO | -12.97 | 0.55 | 13.52 | FeO |
| Ferrite-Ca | -12.91 | 8.59 | 21.50 | CaFe2O4 |
| Ferrite-Cu | -3.60 | 6.68 | 10.28 | CuFe2O4 |
| Ferrite-Dicalcium | -45.96 | 10.84 | 56.80 | Ca2Fe2O5 |
| Ferrite-Mg | -13.28 | 7.74 | 21.02 | MgFe2O4 |
| Ferrite-Zn | -5.64 | 6.06 | 11.70 | ZnFe2O4 |
| FeSO4 | -9.36 | -6.76 | 2.61 | FeSO4 |
| Gibbsite | -4.40 | 3.34 | 7.74 | Al(OH)3 |
| Glauberite | -7.50 | -12.96 | -5.47 | Na2Ca(SO4)2 |
| Goethite | 2.64 | 3.17 | 0.53 | FeOOH |
| Gypsum | -0.53 | -5.06 | -4.53 | CaSO4:2H2O |
| H2(g) | -31.27 | -34.37 | -3.10 | H2 |
| H2O(g) | -1.59 | -0.00 | 1.59 | H2O |
| H2S(g) | -90.69 | -98.68 | -7.99 | H2S |
| Halite | -7.29 | -5.73 | 1.56 | NaCl |
| Hausmannite | -27.61 | -17.46 | 10.14 | Mn3O4 |
| HCl(g) | -11.74 | -5.43 | 6.30 | HCl |
| Hematite | 6.26 | 6.34 | 0.08 | Fe2O3 |
| Hercynite | -21.57 | 7.24 | 28.80 | FeAl2O4 |
| Hexahydrite | -4.18 | -5.90 | -1.73 | MgSO4:6H2O |
| Hydrophilite | -20.36 | -8.62 | 11.75 | CaCl2 |
| Ice | -0.14 | -0.00 | 0.14 | H2O |
| Jarosite | 3.18 | -6.23 | -9.41 | KFe3(SO4)2(OH)6 |
| Jarosite-Na | 0.04 | -5.41 | -5.45 | NaFe3(SO4)2(OH)6 |
| K | -66.23 | 4.75 | 70.98 | K |
| K(g) | -76.83 | 4.75 | 81.58 | K |
| K2O | -86.27 | -2.23 | 84.04 | K2O |
| K3H(SO4)2 | -14.35 | -17.97 | -3.62 | K3H(SO4)2 |
| Kainite | -12.14 | -12.45 | -0.31 | KMgClSO4:3H2O |
| KAl(SO4)2 | -15.67 | -12.39 | 3.27 | KAl(SO4)2 |
| Katoite | -65.51 | 13.43 | 78.94 | Ca3Al2H12O12 |
| Kieserite | -5.64 | -5.90 | -0.27 | MgSO4:H2O |
| KMgCl3 | -37.26 | -16.01 | 21.25 | KMgCl3 |
| KMgCl3:2H2O | -29.97 | -16.01 | 13.96 | KMgCl3:2H2O |
| Lammerite | -16.38 | -14.83 | 1.55 | Cu3(AsO4)2 |
| Lawrencite | -19.37 | -10.31 | 9.05 | FeCl2 |
| Leonite | -11.33 | -15.45 | -4.11 | K2Mg(SO4)2:4H2O |

| | | | | |
|--|---------|---------|--------|---|
| Lime | -30.32 | 2.25 | 32.57 | CaO |
| Magnetite | -3.53 | 6.89 | 10.42 | Fe ₃ O ₄ |
| Manganite | -8.97 | -9.13 | -0.16 | MnO(OH) |
| Manganosite | -17.11 | 0.81 | 17.92 | MnO |
| Mayenite | -420.38 | 73.77 | 494.15 | Ca ₁₂ Al ₁₄ O ₃₃ |
| Melanterite | -4.36 | -6.76 | -2.40 | FeSO ₄ ·7H ₂ O |
| Mercallite | -6.99 | -8.43 | -1.44 | KHSO ₄ |
| Mg | -109.39 | 13.13 | 122.52 | Mg |
| Mg(g) | -129.11 | 13.13 | 142.25 | Mg |
| Mg1.25SO ₄ (OH)0.5:0.5H ₂ O | -10.75 | -5.55 | 5.20 | Mg1.25SO ₄ (OH)0.5:0.5H ₂ O |
| Mg1.5SO ₄ (OH) | -14.41 | -5.20 | 9.21 | Mg1.5SO ₄ (OH) |
| MgCl ₂ :2H ₂ O | -22.19 | -9.46 | 12.73 | MgCl ₂ :2H ₂ O |
| MgCl ₂ :4H ₂ O | -16.76 | -9.46 | 7.30 | MgCl ₂ :4H ₂ O |
| MgCl ₂ :H ₂ O | -25.53 | -9.46 | 16.07 | MgCl ₂ :H ₂ O |
| MgOHCl | -19.92 | -4.03 | 15.89 | MgOHCl |
| MgSO ₄ | -10.73 | -5.90 | 4.83 | MgSO ₄ |
| Mirabilite | -6.75 | -7.91 | -1.15 | Na ₂ SO ₄ :10H ₂ O |
| Misenite | -49.02 | -60.10 | -11.08 | K ₈ H ₆ (SO ₄) ₇ |
| Mn | -70.40 | 12.53 | 82.93 | Mn |
| Mn(OH) ₂ (am) | -14.50 | 0.81 | 15.31 | Mn(OH) ₂ |
| Mn(OH) ₃ | -15.47 | -9.13 | 6.34 | Mn(OH) ₃ |
| MnCl ₂ :2H ₂ O | -14.06 | -10.06 | 4.00 | MnCl ₂ :2H ₂ O |
| MnCl ₂ :4H ₂ O | -12.81 | -10.06 | 2.75 | MnCl ₂ :4H ₂ O |
| MnCl ₂ :H ₂ O | -15.60 | -10.06 | 5.54 | MnCl ₂ :H ₂ O |
| MnO ₂ (gamma) | -11.02 | -27.15 | -16.13 | MnO ₂ |
| MnSO ₄ | -9.11 | -6.50 | 2.61 | MnSO ₄ |
| Molysite | -26.60 | -13.13 | 13.47 | FeCl ₃ |
| Na | -61.80 | 5.57 | 67.37 | Na |
| Na(g) | -75.29 | 5.57 | 80.86 | Na |
| Na ₂ O | -68.01 | -0.60 | 67.42 | Na ₂ O |
| Na ₃ H(SO ₄) ₂ | -14.62 | -15.51 | -0.89 | Na ₃ H(SO ₄) ₂ |
| Na ₄ Ca(SO ₄) ₃ :2H ₂ O | -14.98 | -20.87 | -5.89 | Na ₄ Ca(SO ₄) ₃ :2H ₂ O |
| NaFeO ₂ | -17.01 | 2.87 | 19.88 | NaFeO ₂ |
| Nantokite | -11.22 | -17.99 | -6.77 | CuCl |
| O ₂ (g) | -20.56 | -23.46 | -2.89 | O ₂ |
| Orpiment | -270.01 | -349.49 | -79.49 | As ₂ S ₃ |
| Oxychloride-Mg | -28.45 | -2.62 | 25.83 | Mg ₂ Cl(OH) ₃ :4H ₂ O |
| Pentahydrite | -4.52 | -5.90 | -1.39 | MgSO ₄ :5H ₂ O |
| Periclase | -19.92 | 1.41 | 21.33 | MgO |
| Picromerite | -11.01 | -15.45 | -4.44 | K ₂ Mg(SO ₄) ₂ :6H ₂ O |
| Polyhalite | -11.25 | -25.57 | -14.31 | K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O |
| Portlandite | -20.30 | 2.25 | 22.55 | Ca(OH) ₂ |
| Pyrite | -149.26 | -173.96 | -24.70 | FeS ₂ |
| Pyrolusite | -9.49 | -27.15 | -17.66 | MnO ₂ |
| Pyrrhotite | -94.39 | -98.13 | -3.74 | FeS |
| Realgar | -104.85 | -165.13 | -60.28 | AsS |
| S | -65.30 | -110.41 | -45.11 | S |
| S ₂ (g) | -144.48 | -151.67 | -7.19 | S ₂ |
| Scacchite | -18.80 | -10.06 | 8.74 | MnCl ₂ |
| SO ₂ (g) | -33.26 | -33.09 | 0.18 | SO ₂ |
| Sphalerite | -87.49 | -98.96 | -11.47 | ZnS |
| Spinel | -29.52 | 8.09 | 37.61 | Al ₂ MgO ₄ |
| Starkeyite | -4.90 | -5.90 | -1.00 | MgSO ₄ :4H ₂ O |
| Sylvite | -7.38 | -6.55 | 0.83 | KCl |
| Syngenite | -7.00 | -14.60 | -7.60 | K ₂ Ca(SO ₄) ₂ :H ₂ O |
| Tachyhydrite | -44.69 | -27.54 | 17.14 | Mg ₂ CaCl ₆ :12H ₂ O |
| Tenorite | -7.31 | 0.34 | 7.65 | CuO |
| Thenardite | -7.55 | -7.90 | -0.36 | Na ₂ SO ₄ |
| Todorokite | -64.08 | -109.90 | -45.82 | Mn ₇ O ₁₂ :3H ₂ O |
| Troilite | -94.28 | -98.13 | -3.84 | FeS |
| Wurtzite | -89.79 | -98.96 | -9.17 | ZnS |
| Wustite | -11.60 | 0.80 | 12.40 | Fe ₉₄ 7O |
| Zincite | -11.48 | -0.28 | 11.20 | ZnO |
| Zn | -57.34 | 11.45 | 68.79 | Zn |
| Zn(ClO ₄) ₂ :6H ₂ O | -142.06 | -136.42 | 5.63 | Zn(ClO ₄) ₂ :6H ₂ O |
| Zn(g) | -73.96 | 11.45 | 85.41 | Zn |
| Zn(OH) ₂ (beta) | -12.21 | -0.28 | 11.93 | Zn(OH) ₂ |

| | | | | |
|------------------|--------|--------|-------|-------------|
| Zn(OH)2(epsilon) | -11.94 | -0.28 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -12.16 | -0.28 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -21.28 | -5.99 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -15.44 | -7.86 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -25.99 | -16.68 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -34.54 | -15.45 | 19.09 | Zn3O(SO4)2 |
| ZnCl2 | -18.22 | -11.14 | 7.08 | ZnCl2 |
| ZnSO4 | -11.12 | -7.59 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -5.89 | -7.59 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -5.71 | -7.59 | -1.88 | ZnSO4:7H2O |
| ZnSO4:H2O | -7.04 | -7.59 | -0.55 | ZnSO4:H2O |

End of simulation.

Reading input data for simulation 2.

End of run.
