
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 3
temp 25
pH 3.07
pe 17
redox pe
units mg/l
density 1
Cl 40.91
S(6) 1264
Al 21.6
As 3.82
Ca 124.8
Cu 40.91
Fe 41.51
K 35.01
Mg 13.42
Mn 24.26
Na 20.89
Zn 9.71
C(4) 0
water 1 # kg
SOLUTION 2 AS1
temp 25
units mg/l
pe 10
pH 7.54
Cl 24.2
F 0.25
N(5) 2.9
S(6) 243
Al 0
As 0.0966
Ca 86.82
Cu 0.113
Fe 0
Hg 0
K 3.07
Mg 16.17
Mn 0.181
Na 43.01
Ni 0

```

Pb      0
Zn      0.195
MIX 4
      1      1
      2      1
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 3

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

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

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

```

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

```

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|------------|------------|------------|--------------|--------------|-----------|
| H+ | 9.741e-004 | 8.511e-004 | -3.011 | -3.070 | -0.059 |
| OH- | 1.344e-011 | 1.132e-011 | -10.872 | -10.946 | -0.075 |
| H2O | 5.553e+001 | 9.996e-001 | 1.744 | -0.000 | 0.000 |
| Al | 8.019e-004 | | | | |
| AlSO4+ | 4.097e-004 | 3.464e-004 | -3.388 | -3.460 | -0.073 |
| Al+3 | 2.262e-004 | 6.552e-005 | -3.646 | -4.184 | -0.538 |
| Al(SO4)2- | 1.643e-004 | 1.389e-004 | -3.784 | -3.857 | -0.073 |
| AlOH+2 | 1.676e-006 | 8.621e-007 | -5.776 | -6.064 | -0.289 |
| Al(OH)2+ | 2.781e-009 | 2.351e-009 | -8.556 | -8.629 | -0.073 |
| Al2(OH)2+4 | 1.546e-009 | 1.208e-010 | -8.811 | -9.918 | -1.107 |
| HALO2 | 4.020e-012 | 4.020e-012 | -11.396 | -11.396 | 0.000 |

| | | | | | |
|----------------|------------|------------|----------|----------|--------|
| Al3(OH)4+5 | 3.475e-013 | 7.050e-015 | -12.459 | -14.152 | -1.693 |
| AlO2- | 1.914e-015 | 1.618e-015 | -14.718 | -14.791 | -0.073 |
| NaAlO2 | 2.296e-019 | 2.296e-019 | -18.639 | -18.639 | 0.000 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -51.563 | -54.881 | -3.319 |
| As(-3) | 0.000e+000 | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -151.256 | -151.256 | 0.000 |
| As(3) | 2.419e-026 | | | | |
| HAsO2 | 1.291e-026 | 1.291e-026 | -25.889 | -25.889 | 0.000 |
| As(OH)3 | 1.128e-026 | 1.128e-026 | -25.948 | -25.948 | 0.000 |
| H2AsO3- | 9.588e-033 | 8.107e-033 | -32.018 | -32.091 | -0.073 |
| AsO2- | 9.170e-033 | 7.753e-033 | -32.038 | -32.111 | -0.073 |
| AsO2OH-2 | 1.838e-040 | 0.000e+000 | -39.736 | -40.031 | -0.296 |
| As(5) | 5.107e-005 | | | | |
| H2AsO4- | 4.531e-005 | 3.831e-005 | -4.344 | -4.417 | -0.073 |
| H3AsO4 | 5.743e-006 | 5.743e-006 | -5.241 | -5.241 | 0.000 |
| HAsO4-2 | 1.476e-008 | 7.471e-009 | -7.831 | -8.127 | -0.296 |
| AsO4-3 | 1.045e-016 | 2.252e-017 | -15.981 | -16.647 | -0.667 |
| Ca | 3.119e-003 | | | | |
| Ca+2 | 2.219e-003 | 1.192e-003 | -2.654 | -2.924 | -0.270 |
| CaSO4 | 8.999e-004 | 8.999e-004 | -3.046 | -3.046 | 0.000 |
| CaCl+ | 2.891e-007 | 2.445e-007 | -6.539 | -6.612 | -0.073 |
| CaCl2 | 2.781e-010 | 2.781e-010 | -9.556 | -9.556 | 0.000 |
| CaOH+ | 2.340e-013 | 1.978e-013 | -12.631 | -12.704 | -0.073 |
| Cl(-1) | 1.156e-003 | | | | |
| Cl- | 1.154e-003 | 9.673e-004 | -2.938 | -3.014 | -0.077 |
| CuCl+ | 6.621e-007 | 5.598e-007 | -6.179 | -6.252 | -0.073 |
| MnCl+ | 3.434e-007 | 2.903e-007 | -6.464 | -6.537 | -0.073 |
| CaCl+ | 2.891e-007 | 2.445e-007 | -6.539 | -6.612 | -0.073 |
| HCl | 1.849e-007 | 1.849e-007 | -6.733 | -6.733 | 0.000 |
| MgCl+ | 1.568e-007 | 1.326e-007 | -6.805 | -6.878 | -0.073 |
| NaCl | 1.265e-007 | 1.265e-007 | -6.898 | -6.898 | 0.000 |
| ZnCl+ | 9.697e-008 | 8.198e-008 | -7.013 | -7.086 | -0.073 |
| KCl | 2.345e-008 | 2.345e-008 | -7.630 | -7.630 | 0.000 |
| FeCl+2 | 9.839e-009 | 5.061e-009 | -8.007 | -8.296 | -0.289 |
| FeCl2+ | 4.688e-009 | 3.963e-009 | -8.329 | -8.402 | -0.073 |
| CuCl2 | 2.852e-010 | 2.852e-010 | -9.545 | -9.545 | 0.000 |
| CaCl2 | 2.781e-010 | 2.781e-010 | -9.556 | -9.556 | 0.000 |
| ZnCl2 | 9.263e-011 | 9.263e-011 | -10.033 | -10.033 | 0.000 |
| FeCl+ | 2.730e-012 | 2.308e-012 | -11.564 | -11.637 | -0.073 |
| Zn(OH)Cl | 1.646e-012 | 1.646e-012 | -11.783 | -11.783 | 0.000 |
| MnCl3- | 7.018e-014 | 5.934e-014 | -13.154 | -13.227 | -0.073 |
| ZnCl3- | 5.853e-014 | 4.948e-014 | -13.233 | -13.306 | -0.073 |
| ZnCl4-2 | 7.166e-016 | 3.628e-016 | -15.145 | -15.440 | -0.296 |
| FeCl2 | 1.198e-017 | 1.198e-017 | -16.922 | -16.922 | 0.000 |
| FeCl4- | 5.273e-018 | 4.458e-018 | -17.278 | -17.351 | -0.073 |
| CuCl2- | 8.492e-020 | 7.180e-020 | -19.071 | -19.144 | -0.073 |
| CuCl4-2 | 9.890e-021 | 5.007e-021 | -20.005 | -20.300 | -0.296 |
| CuCl3-2 | 8.809e-022 | 4.460e-022 | -21.055 | -21.351 | -0.296 |
| FeCl4-2 | 6.397e-023 | 3.239e-023 | -22.194 | -22.490 | -0.296 |
| Cl(1) | 3.282e-017 | | | | |
| HClO | 3.282e-017 | 3.282e-017 | -16.484 | -16.484 | 0.000 |
| ClO- | 1.230e-021 | 1.040e-021 | -20.910 | -20.983 | -0.073 |
| Cl(3) | 3.477e-032 | | | | |
| HClO2 | 1.792e-032 | 1.792e-032 | -31.747 | -31.747 | 0.000 |
| ClO2- | 1.685e-032 | 1.424e-032 | -31.773 | -31.846 | -0.073 |
| Cl(5) | 1.650e-029 | | | | |
| ClO3- | 1.650e-029 | 1.389e-029 | -28.783 | -28.857 | -0.075 |
| Cl(7) | 8.035e-031 | | | | |
| ClO4- | 8.027e-031 | 6.758e-031 | -30.095 | -30.170 | -0.075 |
| ZnClO4+ | 7.628e-034 | 6.449e-034 | -33.118 | -33.191 | -0.073 |
| Cu(1) | 1.456e-018 | | | | |
| Cu+ | 1.370e-018 | 1.158e-018 | -17.863 | -17.936 | -0.073 |
| CuCl2- | 8.492e-020 | 7.180e-020 | -19.071 | -19.144 | -0.073 |
| CuCl3-2 | 8.809e-022 | 4.460e-022 | -21.055 | -21.351 | -0.296 |
| Cu(2) | 6.448e-004 | | | | |
| Cu+2 | 3.937e-004 | 2.116e-004 | -3.405 | -3.675 | -0.270 |
| CuSO4 | 2.504e-004 | 2.504e-004 | -3.601 | -3.601 | 0.000 |

| | | | | | |
|------------|------------|------------|---------|---------|--------|
| CuCl+ | 6.621e-007 | 5.598e-007 | -6.179 | -6.252 | -0.073 |
| CuOH+ | 1.516e-008 | 1.282e-008 | -7.819 | -7.892 | -0.073 |
| CuCl2 | 2.852e-010 | 2.852e-010 | -9.545 | -9.545 | 0.000 |
| CuCl4-2 | 9.890e-021 | 5.007e-021 | -20.005 | -20.300 | -0.296 |
| CuO2-2 | 2.825e-031 | 1.430e-031 | -30.549 | -30.845 | -0.296 |
| Fe(2) | 8.779e-009 | | | | |
| Fe+2 | 6.095e-009 | 3.275e-009 | -8.215 | -8.485 | -0.270 |
| FeSO4 | 2.682e-009 | 2.682e-009 | -8.572 | -8.572 | 0.000 |
| FeCl+ | 2.730e-012 | 2.308e-012 | -11.564 | -11.637 | -0.073 |
| FeOH+ | 1.439e-015 | 1.216e-015 | -14.842 | -14.915 | -0.073 |
| FeCl2 | 1.198e-017 | 1.198e-017 | -16.922 | -16.922 | 0.000 |
| FeCl4-2 | 6.397e-023 | 3.239e-023 | -22.194 | -22.490 | -0.296 |
| Fe(OH)2 | 1.135e-023 | 1.135e-023 | -22.945 | -22.945 | 0.000 |
| Fe(OH)3- | 6.276e-031 | 5.306e-031 | -30.202 | -30.275 | -0.073 |
| Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -41.910 | -42.205 | -0.296 |
| Fe(3) | 7.445e-004 | | | | |
| FeOH+2 | 4.629e-004 | 2.381e-004 | -3.335 | -3.623 | -0.289 |
| Fe(OH)2+ | 1.095e-004 | 9.261e-005 | -3.960 | -4.033 | -0.073 |
| Fe+3 | 1.084e-004 | 3.140e-005 | -3.965 | -4.503 | -0.538 |
| Fe2(OH)2+4 | 1.953e-005 | 1.526e-006 | -4.709 | -5.816 | -1.107 |
| FeSO4+ | 1.857e-005 | 1.570e-005 | -4.731 | -4.804 | -0.073 |
| Fe(SO4)2- | 1.622e-006 | 1.371e-006 | -5.790 | -5.863 | -0.073 |
| Fe3(OH)4+5 | 1.455e-006 | 2.953e-008 | -5.837 | -7.530 | -1.693 |
| Fe(OH)3 | 5.087e-008 | 5.087e-008 | -7.294 | -7.294 | 0.000 |
| FeCl+2 | 9.839e-009 | 5.061e-009 | -8.007 | -8.296 | -0.289 |
| FeCl2+ | 4.688e-009 | 3.963e-009 | -8.329 | -8.402 | -0.073 |
| Fe(OH)4- | 1.775e-014 | 1.501e-014 | -13.751 | -13.824 | -0.073 |
| FeCl4- | 5.273e-018 | 4.458e-018 | -17.278 | -17.351 | -0.073 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -43.244 | -43.240 | 0.003 |
| K | 8.969e-004 | | | | |
| K+ | 8.613e-004 | 7.219e-004 | -3.065 | -3.141 | -0.077 |
| KSO4- | 3.561e-005 | 3.011e-005 | -4.448 | -4.521 | -0.073 |
| KCl | 2.345e-008 | 2.345e-008 | -7.630 | -7.630 | 0.000 |
| KHSO4 | 2.261e-008 | 2.261e-008 | -7.646 | -7.646 | 0.000 |
| KOH | 2.940e-015 | 2.940e-015 | -14.532 | -14.532 | 0.000 |
| Mg | 5.531e-004 | | | | |
| Mg+2 | 3.107e-004 | 1.755e-004 | -3.508 | -3.756 | -0.248 |
| MgSO4 | 2.422e-004 | 2.422e-004 | -3.616 | -3.616 | 0.000 |
| MgCl+ | 1.568e-007 | 1.326e-007 | -6.805 | -6.878 | -0.073 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -41.386 | -42.493 | -1.107 |
| Mn(2) | 4.423e-004 | | | | |
| Mn+2 | 2.623e-004 | 1.410e-004 | -3.581 | -3.851 | -0.270 |
| MnSO4 | 1.797e-004 | 1.797e-004 | -3.746 | -3.746 | 0.000 |
| MnCl+ | 3.434e-007 | 2.903e-007 | -6.464 | -6.537 | -0.073 |
| MnOH+ | 5.033e-012 | 4.255e-012 | -11.298 | -11.371 | -0.073 |
| MnCl3- | 7.018e-014 | 5.934e-014 | -13.154 | -13.227 | -0.073 |
| Mn2OH+3 | 2.782e-015 | 6.427e-016 | -14.556 | -15.192 | -0.636 |
| Mn(OH)2 | 1.227e-020 | 1.227e-020 | -19.911 | -19.911 | 0.000 |
| Mn2(OH)3+ | 4.793e-023 | 4.052e-023 | -22.319 | -22.392 | -0.073 |
| Mn(OH)3- | 1.598e-029 | 1.351e-029 | -28.796 | -28.869 | -0.073 |
| Mn(OH)4-2 | 2.655e-040 | 1.344e-040 | -39.576 | -39.872 | -0.296 |
| Mn(3) | 1.627e-012 | | | | |
| Mn+3 | 1.627e-012 | 3.760e-013 | -11.789 | -12.425 | -0.636 |
| Mn(6) | 3.607e-030 | | | | |
| MnO4-2 | 3.607e-030 | 1.826e-030 | -29.443 | -29.738 | -0.296 |
| Mn(7) | 9.551e-023 | | | | |
| MnO4- | 9.551e-023 | 8.041e-023 | -22.020 | -22.095 | -0.075 |
| Na | 9.102e-004 | | | | |
| Na+ | 8.800e-004 | 7.440e-004 | -3.056 | -3.128 | -0.073 |
| NaSO4- | 3.004e-005 | 2.540e-005 | -4.522 | -4.595 | -0.073 |
| NaCl | 1.265e-007 | 1.265e-007 | -6.898 | -6.898 | 0.000 |
| NaOH | 1.452e-015 | 1.452e-015 | -14.838 | -14.838 | 0.000 |
| NaAlO2 | 2.296e-019 | 2.296e-019 | -18.639 | -18.639 | 0.000 |
| O(0) | 3.822e-006 | | | | |
| O2 | 1.911e-006 | 1.926e-006 | -5.719 | -5.715 | 0.003 |
| S(6) | 1.318e-002 | | | | |

| | | | | | |
|-----------|------------|------------|---------|---------|--------|
| SO4-2 | 1.020e-002 | 5.166e-003 | -1.991 | -2.287 | -0.296 |
| CaSO4 | 8.999e-004 | 8.999e-004 | -3.046 | -3.046 | 0.000 |
| HSO4- | 5.254e-004 | 4.442e-004 | -3.280 | -3.352 | -0.073 |
| AlSO4+ | 4.097e-004 | 3.464e-004 | -3.388 | -3.460 | -0.073 |
| CuSO4 | 2.504e-004 | 2.504e-004 | -3.601 | -3.601 | 0.000 |
| MgSO4 | 2.422e-004 | 2.422e-004 | -3.616 | -3.616 | 0.000 |
| MnSO4 | 1.797e-004 | 1.797e-004 | -3.746 | -3.746 | 0.000 |
| Al(SO4)2- | 1.643e-004 | 1.389e-004 | -3.784 | -3.857 | -0.073 |
| ZnSO4 | 5.476e-005 | 5.476e-005 | -4.262 | -4.262 | 0.000 |
| KSO4- | 3.561e-005 | 3.011e-005 | -4.448 | -4.521 | -0.073 |
| NaSO4- | 3.004e-005 | 2.540e-005 | -4.522 | -4.595 | -0.073 |
| FeSO4+ | 1.857e-005 | 1.570e-005 | -4.731 | -4.804 | -0.073 |
| Fe(SO4)2- | 1.622e-006 | 1.371e-006 | -5.790 | -5.863 | -0.073 |
| KHSO4 | 2.261e-008 | 2.261e-008 | -7.646 | -7.646 | 0.000 |
| FeSO4 | 2.682e-009 | 2.682e-009 | -8.572 | -8.572 | 0.000 |
| H2SO4 | 3.567e-010 | 3.567e-010 | -9.448 | -9.448 | 0.000 |
| Zn | 1.487e-004 | | | | |
| Zn+2 | 9.388e-005 | 5.045e-005 | -4.027 | -4.297 | -0.270 |
| ZnSO4 | 5.476e-005 | 5.476e-005 | -4.262 | -4.262 | 0.000 |
| ZnCl+ | 9.697e-008 | 8.198e-008 | -7.013 | -7.086 | -0.073 |
| ZnCl2 | 9.263e-011 | 9.263e-011 | -10.033 | -10.033 | 0.000 |
| ZnOH+ | 7.685e-011 | 6.498e-011 | -10.114 | -10.187 | -0.073 |
| Zn(OH)Cl | 1.646e-012 | 1.646e-012 | -11.783 | -11.783 | 0.000 |
| ZnCl3- | 5.853e-014 | 4.948e-014 | -13.233 | -13.306 | -0.073 |
| ZnCl4-2 | 7.166e-016 | 3.628e-016 | -15.145 | -15.440 | -0.296 |
| Zn(OH)2 | 3.268e-016 | 3.268e-016 | -15.486 | -15.486 | 0.000 |
| Zn(OH)3- | 1.407e-024 | 1.190e-024 | -23.852 | -23.925 | -0.073 |
| ZnClO4+ | 7.628e-034 | 6.449e-034 | -33.118 | -33.191 | -0.073 |
| Zn(OH)4-2 | 4.705e-034 | 2.382e-034 | -33.327 | -33.623 | -0.296 |

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

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

| | | | | |
|--------------------|---------|--------|--------|--------------------------|
| Ca4Al2O7:19H2O | -80.77 | 22.91 | 103.68 | Ca4Al2O7:19H2O |
| Ca4Cl2(OH)6:13H2O | -67.63 | 0.69 | 68.33 | Ca4Cl2(OH)6:13H2O |
| CaAl2O4 | -33.64 | 13.27 | 46.91 | CaAl2O4 |
| CaAl2O4:10H2O | -24.73 | 13.27 | 37.99 | CaAl2O4:10H2O |
| CaAl4O7 | -45.27 | 23.32 | 68.59 | CaAl4O7 |
| Carnallite | -20.21 | -15.94 | 4.27 | KMgCl3:6H2O |
| CaSO4:0.5H2O(beta) | -1.68 | -5.21 | -3.54 | CaSO4:0.5H2O |
| Chalcanthite | -3.33 | -5.96 | -2.63 | CuSO4:5H2O |
| Chalcocyanite | -8.87 | -5.96 | 2.91 | CuSO4 |
| Chloromagnesite | -31.60 | -9.78 | 21.82 | MgCl2 |
| Cl2(g) | -18.02 | -15.03 | 2.99 | Cl2 |
| Claudetite | -50.53 | -70.32 | -19.80 | As2O3 |
| Corundum | -8.24 | 10.05 | 18.29 | Al2O3 |
| Cu | -26.17 | 5.32 | 31.50 | Cu |
| Cu(g) | -78.33 | 5.32 | 83.66 | Cu |
| CuCl2 | -13.42 | -9.70 | 3.72 | CuCl2 |
| Cuprite | -27.83 | -29.73 | -1.91 | Cu2O |
| Delafossite | -3.72 | -10.16 | -6.44 | CuFeO2 |
| Diaspore | -2.12 | 5.03 | 7.15 | AlHO2 |
| Epsomite | -4.08 | -6.04 | -1.96 | MgSO4:7H2O |
| Ettringite | -58.40 | 4.06 | 62.46 | Ca6Al2(SO4)3(OH)12:26H2O |
| Fe | -58.50 | 0.51 | 59.02 | Fe |
| Fe(OH)2 | -16.24 | -2.35 | 13.89 | Fe(OH)2 |
| Fe(OH)3 | -0.93 | 4.71 | 5.64 | Fe(OH)3 |
| Fe2(SO4)3 | -18.91 | -15.87 | 3.05 | Fe2(SO4)3 |
| FeO | -15.87 | -2.34 | 13.52 | FeO |
| Ferrite-Ca | -8.87 | 12.63 | 21.50 | CaFe2O4 |
| Ferrite-Cu | 1.60 | 11.88 | 10.28 | CuFe2O4 |
| Ferrite-Dicalcium | -40.95 | 15.85 | 56.80 | Ca2Fe2O5 |
| Ferrite-Mg | -9.22 | 11.80 | 21.02 | MgFe2O4 |
| Ferrite-Zn | -0.44 | 11.26 | 11.70 | ZnFe2O4 |
| FeSO4 | -13.38 | -10.77 | 2.61 | FeSO4 |
| Gibbsite | -2.71 | 5.03 | 7.74 | Al(OH)3 |
| Glauberite | -8.29 | -13.75 | -5.47 | Na2Ca(SO4)2 |
| Goethite | 4.18 | 4.71 | 0.53 | FeOOH |
| Gypsum | -0.68 | -5.21 | -4.53 | CaSO4:2H2O |
| H2(g) | -40.14 | -43.24 | -3.10 | H2 |
| H2O(g) | -1.59 | -0.00 | 1.59 | H2O |
| Halite | -7.71 | -6.14 | 1.56 | NaCl |
| Hausmannite | -14.29 | -4.14 | 10.14 | Mn3O4 |
| HCl(g) | -12.39 | -6.08 | 6.30 | HCl |
| Hematite | 9.34 | 9.41 | 0.08 | Fe2O3 |
| Hercynite | -21.10 | 7.71 | 28.80 | FeAl2O4 |
| Hexahydrite | -4.32 | -6.04 | -1.73 | MgSO4:6H2O |
| Hydrophilite | -20.70 | -8.95 | 11.75 | CaCl2 |
| Ice | -0.14 | -0.00 | 0.14 | H2O |
| Jarosite | 6.61 | -2.81 | -9.41 | KFe3(SO4)2(OH)6 |
| Jarosite-Na | 2.66 | -2.79 | -5.45 | NaFe3(SO4)2(OH)6 |
| K | -69.62 | 1.36 | 70.98 | K |
| K(g) | -80.22 | 1.36 | 81.58 | K |
| K2O | -84.18 | -0.14 | 84.04 | K2O |
| K3H(SO4)2 | -13.44 | -17.07 | -3.62 | K3H(SO4)2 |
| Kainite | -11.89 | -12.20 | -0.31 | KMgClSO4:3H2O |
| KAl(SO4)2 | -15.17 | -11.90 | 3.27 | KAl(SO4)2 |
| Katoite | -59.24 | 19.70 | 78.94 | Ca3Al2H12O12 |
| Kieserite | -5.78 | -6.04 | -0.27 | MgSO4:H2O |
| KMgCl3 | -37.19 | -15.94 | 21.25 | KMgCl3 |
| KMgCl3:2H2O | -29.90 | -15.94 | 13.96 | KMgCl3:2H2O |
| Lammerite | -9.13 | -7.58 | 1.55 | Cu3(AsO4)2 |
| Lawrencite | -23.57 | -14.51 | 9.05 | FeCl2 |
| Leonite | -10.50 | -14.61 | -4.11 | K2Mg(SO4)2:4H2O |
| Lime | -29.35 | 3.22 | 32.57 | CaO |
| Magnetite | -3.35 | 7.07 | 10.42 | Fe3O4 |
| Manganite | -3.05 | -3.22 | -0.16 | MnO(OH) |
| Manganosite | -15.63 | 2.29 | 17.92 | MnO |
| Mayenite | -385.19 | 108.96 | 494.15 | Ca12Al14O33 |
| Melanterite | -8.37 | -10.77 | -2.40 | FeSO4:7H2O |

| | | | | |
|-------------------------|---------|--------|--------|-------------------------|
| Mercallite | -7.06 | -8.50 | -1.44 | KHSO4 |
| Mg | -117.28 | 5.24 | 122.52 | Mg |
| Mg(g) | -137.00 | 5.24 | 142.25 | Mg |
| Mg1.25SO4(OH)0.5:0.5H2O | -10.64 | -5.45 | 5.20 | Mg1.25SO4(OH)0.5:0.5H2O |
| Mg1.5SO4(OH) | -14.06 | -4.85 | 9.21 | Mg1.5SO4(OH) |
| MgCl2:2H2O | -22.52 | -9.78 | 12.73 | MgCl2:2H2O |
| MgCl2:4H2O | -17.09 | -9.79 | 7.30 | MgCl2:4H2O |
| MgCl2:H2O | -25.86 | -9.78 | 16.07 | MgCl2:H2O |
| MgOHCl | -19.59 | -3.70 | 15.89 | MgOHCl |
| MgSO4 | -10.87 | -6.04 | 4.83 | MgSO4 |
| Mirabilite | -7.39 | -8.55 | -1.15 | Na2SO4:10H2O |
| Misenite | -48.48 | -59.56 | -11.08 | K8H6(SO4)7 |
| Mn | -77.79 | 5.15 | 82.93 | Mn |
| Mn(OH)2(am) | -13.02 | 2.29 | 15.31 | Mn(OH)2 |
| Mn(OH)3 | -9.56 | -3.22 | 6.34 | Mn(OH)3 |
| MnCl2:2H2O | -13.88 | -9.88 | 4.00 | MnCl2:2H2O |
| MnCl2:4H2O | -12.63 | -9.88 | 2.75 | MnCl2:4H2O |
| MnCl2:H2O | -15.42 | -9.88 | 5.54 | MnCl2:H2O |
| MnO2(gamma) | -0.67 | -16.79 | -16.13 | MnO2 |
| MnSO4 | -8.75 | -6.14 | 2.61 | MnSO4 |
| Molysite | -27.02 | -13.55 | 13.47 | FeCl3 |
| Na | -66.00 | 1.37 | 67.37 | Na |
| Na(g) | -79.49 | 1.37 | 80.86 | Na |
| Na2O | -67.53 | -0.12 | 67.42 | Na2O |
| Na3H(SO4)2 | -16.14 | -17.03 | -0.89 | Na3H(SO4)2 |
| Na4Ca(SO4)3:2H2O | -16.40 | -22.30 | -5.89 | Na4Ca(SO4)3:2H2O |
| NaFeO2 | -15.24 | 4.65 | 19.88 | NaFeO2 |
| Nantokite | -14.18 | -20.95 | -6.77 | CuCl |
| O2(g) | -2.82 | -5.72 | -2.89 | O2 |
| Oxychloride-Mg | -27.15 | -1.32 | 25.83 | Mg2Cl(OH)3:4H2O |
| Pentahydrate | -4.66 | -6.04 | -1.39 | MgSO4:5H2O |
| Periclase | -18.94 | 2.38 | 21.33 | MgO |
| Picromerite | -10.17 | -14.61 | -4.44 | K2Mg(SO4)2:6H2O |
| Polyhalite | -10.72 | -25.03 | -14.31 | K2MgCa2(SO4)4:2H2O |
| Portlandite | -19.33 | 3.22 | 22.55 | Ca(OH)2 |
| Pyrolusite | 0.87 | -16.79 | -17.66 | MnO2 |
| Scacchite | -18.62 | -9.88 | 8.74 | MnCl2 |
| Spinel | -25.17 | 12.44 | 37.61 | Al2MgO4 |
| Starkeyite | -5.04 | -6.04 | -1.00 | MgSO4:4H2O |
| Sylvite | -6.98 | -6.16 | 0.83 | KCl |
| Syngenite | -6.18 | -13.78 | -7.60 | K2Ca(SO4)2:H2O |
| Tachyhydrate | -45.67 | -28.52 | 17.14 | Mg2CaCl6:12H2O |
| Tenorite | -5.18 | 2.47 | 7.65 | CuO |
| Thenardite | -8.19 | -8.54 | -0.36 | Na2SO4 |
| Todorokite | -9.35 | -55.17 | -45.82 | Mn7O12:3H2O |
| Wustite | -13.88 | -1.47 | 12.40 | Fe.947O |
| Zincite | -9.36 | 1.84 | 11.20 | ZnO |
| Zn | -64.09 | 4.70 | 68.79 | Zn |
| Zn(ClO4)2:6H2O | -70.27 | -64.64 | 5.63 | Zn(ClO4)2:6H2O |
| Zn(g) | -80.71 | 4.70 | 85.41 | Zn |
| Zn(OH)2(beta) | -10.09 | 1.84 | 11.93 | Zn(OH)2 |
| Zn(OH)2(epsilon) | -9.82 | 1.84 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -10.04 | 1.84 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -17.69 | -2.40 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -12.32 | -4.74 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -18.76 | -9.44 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -30.42 | -11.33 | 19.09 | Zn3O(SO4)2 |
| ZnCl2 | -17.40 | -10.33 | 7.08 | ZnCl2 |
| ZnSO4 | -10.12 | -6.58 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -4.89 | -6.58 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -4.71 | -6.59 | -1.88 | ZnSO4:7H2O |
| ZnSO4:H2O | -6.03 | -6.58 | -0.55 | ZnSO4:H2O |

Initial solution 2. AS1

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

| Elements | Molality | Moles |
|----------|------------|------------|
| As | 1.290e-006 | 1.290e-006 |
| Ca | 2.167e-003 | 2.167e-003 |
| Cl | 6.829e-004 | 6.829e-004 |
| Cu | 1.779e-006 | 1.779e-006 |
| F | 1.316e-005 | 1.316e-005 |
| K | 7.855e-005 | 7.855e-005 |
| Mg | 6.656e-004 | 6.656e-004 |
| Mn | 3.296e-006 | 3.296e-006 |
| N(5) | 2.071e-004 | 2.071e-004 |
| Na | 1.872e-003 | 1.872e-003 |
| S(6) | 2.531e-003 | 2.531e-003 |
| Zn | 2.983e-006 | 2.983e-006 |

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

pH = 7.540
 pe = 10.000
 Activity of water = 1.000
 Ionic strength = 1.056e-002
 Mass of water (kg) = 1.000e+000
 Total alkalinity (eq/kg) = 1.343e-006
 Total carbon (mol/kg) = 0.000e+000
 Total CO2 (mol/kg) = 0.000e+000
 Temperature (deg C) = 25.000
 Electrical balance (eq) = 1.664e-003
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 13.88
 Iterations = 24
 Total H = 1.110507e+002
 Total O = 5.553608e+001

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|----------|------------|------------|--------------|--------------|-----------|
| OH- | 3.718e-007 | 3.340e-007 | -6.430 | -6.476 | -0.047 |
| H+ | 3.161e-008 | 2.884e-008 | -7.500 | -7.540 | -0.040 |
| H2O | 5.553e+001 | 9.999e-001 | 1.744 | -0.000 | 0.000 |
| As(-3) | 0.000e+000 | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -172.417 | -172.417 | 0.000 |
| As(3) | 0.000e+000 | | | | |
| HAsO2 | 0.000e+000 | 0.000e+000 | -62.230 | -62.230 | 0.000 |
| As(OH)3 | 0.000e+000 | 0.000e+000 | -62.288 | -62.288 | 0.000 |
| H2AsO3- | 0.000e+000 | 0.000e+000 | -63.916 | -63.962 | -0.046 |
| AsO2- | 0.000e+000 | 0.000e+000 | -63.936 | -63.981 | -0.046 |
| AsO2OH-2 | 0.000e+000 | 0.000e+000 | -67.247 | -67.432 | -0.185 |
| As(5) | 1.290e-006 | | | | |
| AsO3F-2 | 1.270e-006 | 8.301e-007 | -5.896 | -6.081 | -0.185 |
| HAsO3F- | 1.976e-008 | 1.778e-008 | -7.704 | -7.750 | -0.046 |
| HAsO4-2 | 0.000e+000 | 0.000e+000 | -40.403 | -40.587 | -0.185 |
| H2AsO4- | 0.000e+000 | 0.000e+000 | -41.302 | -41.347 | -0.046 |
| AsO4-3 | 0.000e+000 | 0.000e+000 | -44.222 | -44.638 | -0.416 |
| H3AsO4 | 0.000e+000 | 0.000e+000 | -46.642 | -46.642 | 0.000 |
| Ca | 2.167e-003 | | | | |
| Ca+2 | 1.907e-003 | 1.277e-003 | -2.720 | -2.894 | -0.174 |
| CaSO4 | 2.583e-004 | 2.583e-004 | -3.588 | -3.588 | 0.000 |
| CaNO3+ | 1.313e-006 | 1.181e-006 | -5.882 | -5.928 | -0.046 |
| CaCl+ | 1.840e-007 | 1.656e-007 | -6.735 | -6.781 | -0.046 |
| CaF+ | 7.576e-008 | 6.817e-008 | -7.121 | -7.166 | -0.046 |
| CaOH+ | 6.949e-009 | 6.252e-009 | -8.158 | -8.204 | -0.046 |
| CaCl2 | 1.192e-010 | 1.192e-010 | -9.924 | -9.924 | 0.000 |
| Cl(-1) | 6.829e-004 | | | | |
| Cl- | 6.823e-004 | 6.119e-004 | -3.166 | -3.213 | -0.047 |
| MgCl+ | 1.928e-007 | 1.735e-007 | -6.715 | -6.761 | -0.046 |
| CaCl+ | 1.840e-007 | 1.656e-007 | -6.735 | -6.781 | -0.046 |

| | | | | | |
|------------|------------|------------|---------|---------|--------|
| NaCl | 1.795e-007 | 1.795e-007 | -6.746 | -6.746 | 0.000 |
| MnCl+ | 2.596e-009 | 2.336e-009 | -8.586 | -8.632 | -0.046 |
| ZnCl+ | 1.858e-009 | 1.672e-009 | -8.731 | -8.777 | -0.046 |
| KCl | 1.432e-009 | 1.432e-009 | -8.844 | -8.844 | 0.000 |
| Zn(OH)Cl | 9.910e-010 | 9.910e-010 | -9.004 | -9.004 | 0.000 |
| CuCl+ | 8.707e-010 | 7.835e-010 | -9.060 | -9.106 | -0.046 |
| CaCl2 | 1.192e-010 | 1.192e-010 | -9.924 | -9.924 | 0.000 |
| HCl | 3.964e-012 | 3.964e-012 | -11.402 | -11.402 | 0.000 |
| ZnCl2 | 1.195e-012 | 1.195e-012 | -11.923 | -11.923 | 0.000 |
| CuCl2 | 2.525e-013 | 2.525e-013 | -12.598 | -12.598 | 0.000 |
| CuCl2- | 7.065e-016 | 6.357e-016 | -15.151 | -15.197 | -0.046 |
| ZnCl3- | 4.488e-016 | 4.039e-016 | -15.348 | -15.394 | -0.046 |
| MnCl3- | 2.124e-016 | 1.911e-016 | -15.673 | -15.719 | -0.046 |
| CuCl3-2 | 3.823e-018 | 2.498e-018 | -17.418 | -17.602 | -0.185 |
| ZnCl4-2 | 2.866e-018 | 1.873e-018 | -17.543 | -17.727 | -0.185 |
| CuCl4-2 | 2.715e-024 | 1.774e-024 | -23.566 | -23.751 | -0.185 |
| Cl(1) | 1.250e-026 | | | | |
| ClO- | 6.368e-027 | 5.730e-027 | -26.196 | -26.242 | -0.046 |
| HClO | 6.129e-027 | 6.129e-027 | -26.213 | -26.213 | 0.000 |
| Cl(3) | 0.000e+000 | | | | |
| ClO2- | 0.000e+000 | 0.000e+000 | -42.119 | -42.165 | -0.046 |
| HClO2 | 0.000e+000 | 0.000e+000 | -46.535 | -46.535 | 0.000 |
| Cl(5) | 0.000e+000 | | | | |
| ClO3- | 0.000e+000 | 0.000e+000 | -44.189 | -44.236 | -0.047 |
| Cl(7) | 0.000e+000 | | | | |
| ClO4- | 0.000e+000 | 0.000e+000 | -50.562 | -50.609 | -0.047 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -55.075 | -55.121 | -0.046 |
| Cu(1) | 2.919e-014 | | | | |
| Cu+ | 2.848e-014 | 2.562e-014 | -13.546 | -13.591 | -0.046 |
| CuCl2- | 7.065e-016 | 6.357e-016 | -15.151 | -15.197 | -0.046 |
| CuCl3-2 | 3.823e-018 | 2.498e-018 | -17.418 | -17.602 | -0.185 |
| Cu(2) | 1.779e-006 | | | | |
| CuOH+ | 9.303e-007 | 8.370e-007 | -6.031 | -6.077 | -0.046 |
| Cu+2 | 6.992e-007 | 4.681e-007 | -6.155 | -6.330 | -0.174 |
| CuSO4 | 1.485e-007 | 1.485e-007 | -6.828 | -6.828 | 0.000 |
| CuCl+ | 8.707e-010 | 7.835e-010 | -9.060 | -9.106 | -0.046 |
| CuF+ | 8.661e-011 | 7.793e-011 | -10.062 | -10.108 | -0.046 |
| CuCl2 | 2.525e-013 | 2.525e-013 | -12.598 | -12.598 | 0.000 |
| CuO2-2 | 3.675e-016 | 2.402e-016 | -15.435 | -15.620 | -0.185 |
| CuCl4-2 | 2.715e-024 | 1.774e-024 | -23.566 | -23.751 | -0.185 |
| F | 1.316e-005 | | | | |
| F- | 1.169e-005 | 1.050e-005 | -4.932 | -4.979 | -0.047 |
| AsO3F-2 | 1.270e-006 | 8.301e-007 | -5.896 | -6.081 | -0.185 |
| MgF+ | 1.023e-007 | 9.206e-008 | -6.990 | -7.036 | -0.046 |
| CaF+ | 7.576e-008 | 6.817e-008 | -7.121 | -7.166 | -0.046 |
| HAsO3F- | 1.976e-008 | 1.778e-008 | -7.704 | -7.750 | -0.046 |
| NaF | 1.875e-009 | 1.875e-009 | -8.727 | -8.727 | 0.000 |
| MnF+ | 5.633e-010 | 5.068e-010 | -9.249 | -9.295 | -0.046 |
| HF | 4.651e-010 | 4.651e-010 | -9.332 | -9.332 | 0.000 |
| ZnF+ | 2.681e-010 | 2.413e-010 | -9.572 | -9.617 | -0.046 |
| CuF+ | 8.661e-011 | 7.793e-011 | -10.062 | -10.108 | -0.046 |
| HF2- | 1.315e-015 | 1.183e-015 | -14.881 | -14.927 | -0.046 |
| H2F2 | 5.380e-019 | 5.380e-019 | -18.269 | -18.269 | 0.000 |
| H(0) | 1.317e-038 | | | | |
| H2 | 6.583e-039 | 6.600e-039 | -38.182 | -38.180 | 0.001 |
| K | 7.855e-005 | | | | |
| K+ | 7.769e-005 | 6.967e-005 | -4.110 | -4.157 | -0.047 |
| KSO4- | 8.657e-007 | 7.790e-007 | -6.063 | -6.108 | -0.046 |
| KCl | 1.432e-009 | 1.432e-009 | -8.844 | -8.844 | 0.000 |
| KOH | 8.375e-012 | 8.375e-012 | -11.077 | -11.077 | 0.000 |
| KHSO4 | 1.982e-014 | 1.982e-014 | -13.703 | -13.703 | 0.000 |
| Mg | 6.656e-004 | | | | |
| Mg+2 | 5.310e-004 | 3.631e-004 | -3.275 | -3.440 | -0.165 |
| MgSO4 | 1.343e-004 | 1.343e-004 | -3.872 | -3.872 | 0.000 |
| MgCl+ | 1.928e-007 | 1.735e-007 | -6.715 | -6.761 | -0.046 |
| MgF+ | 1.023e-007 | 9.206e-008 | -6.990 | -7.036 | -0.046 |
| Mg4(OH)4+4 | 2.283e-023 | 4.466e-024 | -22.642 | -23.350 | -0.709 |

| | | | | | | |
|-----------|------------|------------|---------|---------|--------|--|
| Mn(2) | 3.296e-006 | | | | | |
| Mn+2 | 2.678e-006 | 1.793e-006 | -5.572 | -5.747 | -0.174 | |
| MnSO4 | 6.126e-007 | 6.126e-007 | -6.213 | -6.213 | 0.000 | |
| MnCl+ | 2.596e-009 | 2.336e-009 | -8.586 | -8.632 | -0.046 | |
| MnOH+ | 1.775e-009 | 1.597e-009 | -8.751 | -8.797 | -0.046 | |
| MnNO3+ | 5.828e-010 | 5.244e-010 | -9.234 | -9.280 | -0.046 | |
| MnF+ | 5.633e-010 | 5.068e-010 | -9.249 | -9.295 | -0.046 | |
| Mn(NO3)2 | 2.432e-013 | 2.432e-013 | -12.614 | -12.614 | 0.000 | |
| Mn2(OH)3+ | 1.873e-013 | 1.686e-013 | -12.727 | -12.773 | -0.046 | |
| Mn(OH)2 | 1.359e-013 | 1.359e-013 | -12.867 | -12.867 | 0.000 | |
| Mn2OH+3 | 7.780e-015 | 3.068e-015 | -14.109 | -14.513 | -0.404 | |
| MnCl3- | 2.124e-016 | 1.911e-016 | -15.673 | -15.719 | -0.046 | |
| Mn(OH)3- | 4.913e-018 | 4.421e-018 | -17.309 | -17.355 | -0.046 | |
| Mn(OH)4-2 | 1.986e-024 | 1.298e-024 | -23.702 | -23.887 | -0.185 | |
| Mn(3) | 1.212e-021 | | | | | |
| Mn+3 | 1.212e-021 | 4.781e-022 | -20.916 | -21.320 | -0.404 | |
| Mn(6) | 2.047e-024 | | | | | |
| MnO4-2 | 2.047e-024 | 1.338e-024 | -23.689 | -23.874 | -0.185 | |
| Mn(7) | 6.557e-024 | | | | | |
| MnO4- | 6.557e-024 | 5.890e-024 | -23.183 | -23.230 | -0.047 | |
| N(5) | 2.071e-004 | | | | | |
| NO3- | 2.058e-004 | 1.846e-004 | -3.687 | -3.734 | -0.047 | |
| CaNO3+ | 1.313e-006 | 1.181e-006 | -5.882 | -5.928 | -0.046 | |
| MnNO3+ | 5.828e-010 | 5.244e-010 | -9.234 | -9.280 | -0.046 | |
| HNO3 | 2.784e-013 | 2.784e-013 | -12.555 | -12.555 | 0.000 | |
| Mn(NO3)2 | 2.432e-013 | 2.432e-013 | -12.614 | -12.614 | 0.000 | |
| Na | 1.872e-003 | | | | | |
| Na+ | 1.854e-003 | 1.669e-003 | -2.732 | -2.778 | -0.046 | |
| NaSO4- | 1.697e-005 | 1.527e-005 | -4.770 | -4.816 | -0.046 | |
| NaCl | 1.795e-007 | 1.795e-007 | -6.746 | -6.746 | 0.000 | |
| NaF | 1.875e-009 | 1.875e-009 | -8.727 | -8.727 | 0.000 | |
| NaOH | 9.616e-011 | 9.616e-011 | -10.017 | -10.017 | 0.000 | |
| O(0) | 2.916e-016 | | | | | |
| O2 | 1.458e-016 | 1.462e-016 | -15.836 | -15.835 | 0.001 | |
| S(6) | 2.531e-003 | | | | | |
| SO4-2 | 2.119e-003 | 1.385e-003 | -2.674 | -2.858 | -0.185 | |
| CaSO4 | 2.583e-004 | 2.583e-004 | -3.588 | -3.588 | 0.000 | |
| MgSO4 | 1.343e-004 | 1.343e-004 | -3.872 | -3.872 | 0.000 | |
| NaSO4- | 1.697e-005 | 1.527e-005 | -4.770 | -4.816 | -0.046 | |
| KSO4- | 8.657e-007 | 7.790e-007 | -6.063 | -6.108 | -0.046 | |
| MnSO4 | 6.126e-007 | 6.126e-007 | -6.213 | -6.213 | 0.000 | |
| ZnSO4 | 4.733e-007 | 4.733e-007 | -6.325 | -6.325 | 0.000 | |
| CuSO4 | 1.485e-007 | 1.485e-007 | -6.828 | -6.828 | 0.000 | |
| HSO4- | 4.485e-009 | 4.035e-009 | -8.348 | -8.394 | -0.046 | |
| KHSO4 | 1.982e-014 | 1.982e-014 | -13.703 | -13.703 | 0.000 | |
| H2SO4 | 1.098e-019 | 1.098e-019 | -18.959 | -18.959 | 0.000 | |
| Zn | 2.983e-006 | | | | | |
| Zn+2 | 2.429e-006 | 1.626e-006 | -5.615 | -5.789 | -0.174 | |
| ZnSO4 | 4.733e-007 | 4.733e-007 | -6.325 | -6.325 | 0.000 | |
| ZnOH+ | 6.871e-008 | 6.182e-008 | -7.163 | -7.209 | -0.046 | |
| Zn(OH)2 | 9.179e-009 | 9.179e-009 | -8.037 | -8.037 | 0.000 | |
| ZnCl+ | 1.858e-009 | 1.672e-009 | -8.731 | -8.777 | -0.046 | |
| Zn(OH)Cl | 9.910e-010 | 9.910e-010 | -9.004 | -9.004 | 0.000 | |
| ZnF+ | 2.681e-010 | 2.413e-010 | -9.572 | -9.617 | -0.046 | |
| ZnCl2 | 1.195e-012 | 1.195e-012 | -11.923 | -11.923 | 0.000 | |
| Zn(OH)3- | 1.096e-012 | 9.864e-013 | -11.960 | -12.006 | -0.046 | |
| ZnCl3- | 4.488e-016 | 4.039e-016 | -15.348 | -15.394 | -0.046 | |
| Zn(OH)4-2 | 8.921e-018 | 5.830e-018 | -17.050 | -17.234 | -0.185 | |
| ZnCl4-2 | 2.866e-018 | 1.873e-018 | -17.543 | -17.727 | -0.185 | |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -55.075 | -55.121 | -0.046 | |

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

| Phase | SI | log IAP | log KT | |
|--------------|--------|---------|--------|------------|
| Anhydrite | -1.40 | -5.75 | -4.35 | CaSO4 |
| Antarcticite | -13.41 | -9.32 | 4.09 | CaCl2:6H2O |

| | | | | |
|---|---------|---------|--------|---|
| Antlerite | -0.42 | 8.31 | 8.73 | Cu ₃ (SO ₄)(OH) ₄ |
| Aphthitalite | -17.08 | -20.97 | -3.89 | NaK ₃ (SO ₄) ₂ |
| Arcanite | -9.33 | -11.17 | -1.84 | K ₂ SO ₄ |
| Arsenolite | -123.16 | -143.00 | -19.84 | As ₂ O ₃ |
| As | -102.31 | -59.63 | 42.68 | As |
| As ₂ O ₅ | -99.91 | -97.77 | 2.14 | As ₂ O ₅ |
| As ₄ O ₆ (cubi) | -246.18 | -286.01 | -39.82 | As ₄ O ₆ |
| As ₄ O ₆ (mono) | -245.96 | -286.01 | -40.05 | As ₄ O ₆ |
| Atacamite | -0.77 | 13.49 | 14.26 | Cu ₄ Cl ₂ (OH) ₆ |
| Bassanite | -2.05 | -5.75 | -3.71 | CaSO ₄ :0.5H ₂ O |
| Birnessite | 15.35 | -70.19 | -85.55 | Mn ₈ O ₁₄ :5H ₂ O |
| Bischofite | -14.26 | -9.87 | 4.39 | MgCl ₂ :6H ₂ O |
| Bixbyite | 3.56 | 2.60 | -0.96 | Mn ₂ O ₃ |
| Bloedite | -12.23 | -14.71 | -2.48 | Na ₂ Mg(SO ₄) ₂ :4H ₂ O |
| Brochantite | 1.64 | 17.06 | 15.42 | Cu ₄ (SO ₄)(OH) ₆ |
| Brucite | -4.64 | 11.64 | 16.28 | Mg(OH) ₂ |
| Ca | -119.73 | 20.10 | 139.83 | Ca |
| Ca(g) | -144.97 | 20.10 | 165.07 | Ca |
| Ca ₂ Cl ₂ (OH) ₂ :H ₂ O | -23.42 | 2.87 | 26.29 | Ca ₂ Cl ₂ (OH) ₂ :H ₂ O |
| Ca ₃ (AsO ₄) ₂ | -79.02 | -61.22 | 17.80 | Ca ₃ (AsO ₄) ₂ |
| Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O | -41.09 | 27.24 | 68.33 | Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O |
| Carnallite | -21.51 | -17.24 | 4.27 | KMgCl ₃ :6H ₂ O |
| CaSO ₄ :0.5H ₂ O(beta) | -2.22 | -5.75 | -3.54 | CaSO ₄ :0.5H ₂ O |
| Chalcanthite | -6.56 | -9.19 | -2.63 | CuSO ₄ :5H ₂ O |
| Chalcocyanite | -12.10 | -9.19 | 2.91 | CuSO ₄ |
| Chloromagnesite | -31.68 | -9.87 | 21.82 | MgCl ₂ |
| Cl ₂ (g) | -32.42 | -29.42 | 2.99 | Cl ₂ |
| Claudetite | -123.21 | -143.00 | -19.80 | As ₂ O ₃ |
| Cu | -14.83 | 16.67 | 31.50 | Cu |
| Cu(g) | -66.99 | 16.67 | 83.66 | Cu |
| CuCl ₂ | -16.48 | -12.76 | 3.72 | CuCl ₂ |
| CuF | -25.65 | -18.57 | 7.08 | CuF |
| CuF ₂ | -15.67 | -16.29 | -0.62 | CuF ₂ |
| CuF ₂ :2H ₂ O | -11.74 | -16.29 | -4.55 | CuF ₂ :2H ₂ O |
| Cuprite | -10.20 | -12.10 | -1.91 | Cu ₂ O |
| Epsomite | -4.34 | -6.30 | -1.96 | MgSO ₄ :7H ₂ O |
| F ₂ (g) | -88.67 | -32.95 | 55.71 | F ₂ |
| Fluorite | -2.78 | -12.85 | -10.07 | CaF ₂ |
| Glauberite | -8.70 | -14.17 | -5.47 | Na ₂ Ca(SO ₄) ₂ |
| Gypsum | -1.22 | -5.75 | -4.53 | CaSO ₄ :2H ₂ O |
| H ₂ (g) | -35.08 | -38.18 | -3.10 | H ₂ |
| H ₂ O(g) | -1.59 | -0.00 | 1.59 | H ₂ O |
| Halite | -7.55 | -5.99 | 1.56 | NaCl |
| Hausmannite | 1.79 | 11.93 | 10.14 | Mn ₃ O ₄ |
| HCl(g) | -17.06 | -10.75 | 6.30 | HCl |
| Hexahydrite | -4.57 | -6.30 | -1.73 | MgSO ₄ :6H ₂ O |
| Hydrophilite | -21.07 | -9.32 | 11.75 | CaCl ₂ |
| Ice | -0.14 | -0.00 | 0.14 | H ₂ O |
| K | -63.63 | 7.34 | 70.98 | K |
| K(g) | -74.24 | 7.34 | 81.58 | K |
| K ₂ O | -77.27 | 6.77 | 84.04 | K ₂ O |
| K ₃ H(SO ₄) ₂ | -22.10 | -25.73 | -3.62 | K ₃ H(SO ₄) ₂ |
| Kainite | -13.36 | -13.67 | -0.31 | KMgClSO ₄ :3H ₂ O |
| Kieserite | -6.03 | -6.30 | -0.27 | MgSO ₄ :H ₂ O |
| KMgCl ₃ | -38.48 | -17.24 | 21.25 | KMgCl ₃ |
| KMgCl ₃ :2H ₂ O | -31.20 | -17.24 | 13.96 | KMgCl ₃ :2H ₂ O |
| Lammerite | -73.08 | -71.52 | 1.55 | Cu ₃ (AsO ₄) ₂ |
| Leonite | -13.36 | -17.47 | -4.11 | K ₂ Mg(SO ₄) ₂ :4H ₂ O |
| Lime | -20.38 | 12.19 | 32.57 | CaO |
| Manganite | 1.46 | 1.30 | -0.16 | MnO(OH) |
| Manganosite | -8.58 | 9.33 | 17.92 | MnO |
| Mercallite | -13.12 | -14.56 | -1.44 | KHSO ₄ |
| Mg | -102.96 | 19.56 | 122.52 | Mg |
| Mg(g) | -122.69 | 19.56 | 142.25 | Mg |
| Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O | -8.58 | -3.39 | 5.20 | Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O |
| Mg _{1.5} SO ₄ (OH) | -9.69 | -0.48 | 9.21 | Mg _{1.5} SO ₄ (OH) |
| MgCl ₂ :2H ₂ O | -22.60 | -9.87 | 12.73 | MgCl ₂ :2H ₂ O |

| | | | | |
|------------------|---------|---------|--------|--------------------|
| MgCl2:4H2O | -17.17 | -9.87 | 7.30 | MgCl2:4H2O |
| MgCl2:H2O | -25.94 | -9.87 | 16.07 | MgCl2:H2O |
| MgOHCl | -15.00 | 0.89 | 15.89 | MgOHCl |
| MgSO4 | -11.13 | -6.30 | 4.83 | MgSO4 |
| Mirabilite | -7.26 | -8.41 | -1.15 | Na2SO4:10H2O |
| Misenite | -87.43 | -98.50 | -11.08 | K8H6(SO4)7 |
| Mn | -65.68 | 17.25 | 82.93 | Mn |
| Mn(OH)2(am) | -5.97 | 9.33 | 15.31 | Mn(OH)2 |
| Mn(OH)3 | -5.04 | 1.30 | 6.34 | Mn(OH)3 |
| MnCl2:2H2O | -16.17 | -12.17 | 4.00 | MnCl2:2H2O |
| MnCl2:4H2O | -14.92 | -12.17 | 2.75 | MnCl2:4H2O |
| MnCl2:H2O | -17.71 | -12.17 | 5.54 | MnCl2:H2O |
| MnO2(gamma) | 1.32 | -14.81 | -16.13 | MnO2 |
| MnSO4 | -11.21 | -8.61 | 2.61 | MnSO4 |
| Na | -58.65 | 8.72 | 67.37 | Na |
| Na(g) | -72.14 | 8.72 | 80.86 | Na |
| Na2O | -57.89 | 9.52 | 67.42 | Na2O |
| Na3H(SO4)2 | -20.70 | -21.59 | -0.89 | Na3H(SO4)2 |
| Na4Ca(SO4)3:2H2O | -16.69 | -22.58 | -5.89 | Na4Ca(SO4)3:2H2O |
| Nantokite | -10.04 | -16.80 | -6.77 | CuCl |
| Niter | -7.67 | -7.89 | -0.22 | KNO3 |
| NO2(g) | -15.66 | -7.31 | 8.35 | NO2 |
| O2(g) | -12.94 | -15.84 | -2.89 | O2 |
| Oxychloride-Mg | -13.31 | 12.53 | 25.83 | Mg2Cl(OH)3:4H2O |
| Pentahydrate | -4.91 | -6.30 | -1.39 | MgSO4:5H2O |
| Periclase | -9.69 | 11.64 | 21.33 | MgO |
| Picromerite | -13.03 | -17.47 | -4.44 | K2Mg(SO4)2:6H2O |
| Polyhalite | -14.66 | -28.98 | -14.31 | K2MgCa2(SO4)4:2H2O |
| Portlandite | -10.36 | 12.19 | 22.55 | Ca(OH)2 |
| Pyrolusite | 2.85 | -14.81 | -17.66 | MnO2 |
| Scacchite | -20.91 | -12.17 | 8.74 | MnCl2 |
| Sellaite | -3.95 | -13.40 | -9.44 | MgF2 |
| Starkeyite | -5.30 | -6.30 | -1.00 | MgSO4:4H2O |
| Sylvite | -8.20 | -7.37 | 0.83 | KCl |
| Syngenite | -9.32 | -16.92 | -7.60 | K2Ca(SO4)2:H2O |
| Tachyhydrite | -46.20 | -29.05 | 17.14 | Mg2CaCl6:12H2O |
| Tenorite | 1.10 | 8.75 | 7.65 | CuO |
| Thenardite | -8.06 | -8.41 | -0.36 | Na2SO4 |
| Todorokite | 14.67 | -31.16 | -45.82 | Mn7O12:3H2O |
| Zincite | -1.91 | 9.29 | 11.20 | ZnO |
| Zn | -51.58 | 17.21 | 68.79 | Zn |
| Zn(ClO4)2:6H2O | -112.64 | -107.01 | 5.63 | Zn(ClO4)2:6H2O |
| Zn(g) | -68.20 | 17.21 | 85.41 | Zn |
| Zn(NO3)2:6H2O | -16.66 | -13.26 | 3.40 | Zn(NO3)2:6H2O |
| Zn(OH)2(beta) | -2.64 | 9.29 | 11.93 | Zn(OH)2 |
| Zn(OH)2(epsilon) | -2.37 | 9.29 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -2.59 | 9.29 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -7.46 | 7.83 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -6.94 | 0.64 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -79.21 | -69.90 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -27.09 | -8.00 | 19.09 | Zn3O(SO4)2 |
| Zn5(NO3)2(OH)8 | -18.76 | 23.91 | 42.67 | Zn5(NO3)2(OH)8 |
| ZnCl2 | -19.29 | -12.22 | 7.08 | ZnCl2 |
| ZnF2 | -15.25 | -15.75 | -0.49 | ZnF2 |
| ZnSO4 | -12.18 | -8.65 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -6.95 | -8.65 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -6.77 | -8.65 | -1.88 | ZnSO4:7H2O |
| ZnSO4:H2O | -8.10 | -8.65 | -0.55 | ZnSO4:H2O |

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 4.

Mixture 4.

1.000e+000 Solution 1 Flujo 3
1.000e+000 Solution 2 AS1

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

| Elements | Molality | Moles |
|----------|------------|------------|
| Al | 4.009e-004 | 8.019e-004 |
| As | 2.618e-005 | 5.236e-005 |
| Ca | 2.643e-003 | 5.286e-003 |
| Cl | 9.194e-004 | 1.839e-003 |
| Cu | 3.233e-004 | 6.466e-004 |
| F | 6.582e-006 | 1.316e-005 |
| Fe | 3.723e-004 | 7.445e-004 |
| K | 4.877e-004 | 9.755e-004 |
| Mg | 6.093e-004 | 1.219e-003 |
| Mn | 2.228e-004 | 4.456e-004 |
| N | 1.036e-004 | 2.071e-004 |
| Na | 1.391e-003 | 2.782e-003 |
| S | 7.857e-003 | 1.571e-002 |
| Zn | 7.586e-005 | 1.517e-004 |

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

| | | | |
|--|---|---------------|-------------------------------|
| pH | = | 3.276 | Charge balance |
| pe | = | 16.729 | Adjusted to redox equilibrium |
| Activity of water | = | 1.000 | |
| Ionic strength | = | 2.151e-002 | |
| Mass of water (kg) | = | 2.000e+000 | |
| Total alkalinity (eq/kg) | = | -1.132e-003 | |
| Total carbon (mol/kg) | = | 0.000e+000 | |
| Total CO2 (mol/kg) | = | 0.000e+000 | |
| Temperature (deg C) | = | 25.000 | |
| Electrical balance (eq) | = | -8.870e-003 | |
| Percent error, 100*(Cat- An)/(Cat+ An) | = | -19.05 | |
| Iterations | = | 50 | |
| Total H | = | 2.221036e+002 | |
| Total O | = | 1.111151e+002 | |

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|----------------|------------|------------|--------------|--------------|-----------|
| H+ | 5.961e-004 | 5.295e-004 | -3.225 | -3.276 | -0.051 |
| OH- | 2.104e-011 | 1.819e-011 | -10.677 | -10.740 | -0.063 |
| H2O | 5.553e+001 | 9.998e-001 | 1.744 | -0.000 | 0.000 |
| Al | 4.009e-004 | | | | |
| AlSO4+ | 2.011e-004 | 1.743e-004 | -3.697 | -3.759 | -0.062 |
| Al+3 | 1.433e-004 | 4.856e-005 | -3.844 | -4.314 | -0.470 |
| Al(SO4)2- | 5.476e-005 | 4.747e-005 | -4.262 | -4.324 | -0.062 |
| AlOH+2 | 1.808e-006 | 1.027e-006 | -5.743 | -5.988 | -0.246 |
| Al(OH)2+ | 5.194e-009 | 4.503e-009 | -8.285 | -8.347 | -0.062 |
| Al2(OH)2+4 | 1.521e-009 | 1.716e-010 | -8.818 | -9.766 | -0.948 |
| HALO2 | 1.237e-011 | 1.237e-011 | -10.907 | -10.907 | 0.000 |
| Al3(OH)4+5 | 5.446e-013 | 1.917e-014 | -12.264 | -13.717 | -1.453 |
| AlO2- | 9.233e-015 | 8.005e-015 | -14.035 | -14.097 | -0.062 |
| NaAlO2 | 1.800e-018 | 1.800e-018 | -17.745 | -17.745 | 0.000 |
| AlF+2 | 0.000e+000 | 0.000e+000 | -40.349 | -40.595 | -0.246 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -47.126 | -49.976 | -2.850 |
| AlF2+ | 0.000e+000 | 0.000e+000 | -78.214 | -78.276 | -0.062 |
| AlF3 | 0.000e+000 | 0.000e+000 | -117.458 | -117.458 | 0.000 |
| AlF4- | 0.000e+000 | 0.000e+000 | -158.277 | -158.339 | -0.062 |
| As(-3) | 0.000e+000 | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -151.331 | -151.331 | 0.000 |

| | | | | | | |
|----------|------------|------------|----------|----------|--------|--|
| As (3) | 8.316e-027 | | | | | |
| HAsO2 | 4.437e-027 | 4.437e-027 | -26.353 | -26.353 | 0.000 | |
| As(OH)3 | 3.879e-027 | 3.879e-027 | -26.411 | -26.411 | 0.000 | |
| H2AsO3- | 5.167e-033 | 4.480e-033 | -32.287 | -32.349 | -0.062 | |
| AsO2- | 4.941e-033 | 4.284e-033 | -32.306 | -32.368 | -0.062 | |
| AsO2OH-2 | 1.472e-040 | 0.000e+000 | -39.832 | -40.083 | -0.251 | |
| HAsS2 | 0.000e+000 | 0.000e+000 | -275.826 | -275.826 | 0.000 | |
| As (5) | 2.618e-005 | | | | | |
| H2AsO4- | 1.812e-005 | 1.571e-005 | -4.742 | -4.804 | -0.062 | |
| HAsO3F- | 6.557e-006 | 5.684e-006 | -5.183 | -5.245 | -0.062 | |
| H3AsO4 | 1.466e-006 | 1.466e-006 | -5.834 | -5.834 | 0.000 | |
| AsO3F-2 | 2.575e-008 | 1.446e-008 | -7.589 | -7.840 | -0.251 | |
| HAsO4-2 | 8.772e-009 | 4.925e-009 | -8.057 | -8.308 | -0.251 | |
| AsO4-3 | 8.764e-017 | 2.386e-017 | -16.057 | -16.622 | -0.565 | |
| Ca | 2.643e-003 | | | | | |
| Ca+2 | 2.032e-003 | 1.191e-003 | -2.692 | -2.924 | -0.232 | |
| CaSO4 | 6.105e-004 | 6.105e-004 | -3.214 | -3.214 | 0.000 | |
| CaNO3+ | 6.103e-007 | 5.292e-007 | -6.214 | -6.276 | -0.062 | |
| CaCl+ | 2.304e-007 | 1.998e-007 | -6.637 | -6.699 | -0.062 | |
| CaCl2 | 1.859e-010 | 1.859e-010 | -9.731 | -9.731 | 0.000 | |
| CaOH+ | 3.665e-013 | 3.177e-013 | -12.436 | -12.498 | -0.062 | |
| CaF+ | 0.000e+000 | 0.000e+000 | -45.437 | -45.499 | -0.062 | |
| Cl (-1) | 9.194e-004 | | | | | |
| Cl- | 9.181e-004 | 7.912e-004 | -3.037 | -3.102 | -0.065 | |
| CuCl+ | 3.213e-007 | 2.786e-007 | -6.493 | -6.555 | -0.062 | |
| CaCl+ | 2.304e-007 | 1.998e-007 | -6.637 | -6.699 | -0.062 | |
| MnCl+ | 1.683e-007 | 1.459e-007 | -6.774 | -6.836 | -0.062 | |
| MgCl+ | 1.682e-007 | 1.458e-007 | -6.774 | -6.836 | -0.062 | |
| NaCl | 1.639e-007 | 1.639e-007 | -6.786 | -6.786 | 0.000 | |
| HCl | 9.410e-008 | 9.410e-008 | -7.026 | -7.026 | 0.000 | |
| ZnCl+ | 4.759e-008 | 4.126e-008 | -7.322 | -7.384 | -0.062 | |
| KCl | 1.086e-008 | 1.086e-008 | -7.964 | -7.964 | 0.000 | |
| FeCl+2 | 2.508e-009 | 1.424e-009 | -8.601 | -8.846 | -0.246 | |
| FeCl2+ | 1.052e-009 | 9.123e-010 | -8.978 | -9.040 | -0.062 | |
| CaCl2 | 1.859e-010 | 1.859e-010 | -9.731 | -9.731 | 0.000 | |
| CuCl2 | 1.161e-010 | 1.161e-010 | -9.935 | -9.935 | 0.000 | |
| ZnCl2 | 3.813e-011 | 3.813e-011 | -10.419 | -10.419 | 0.000 | |
| FeCl+ | 1.398e-012 | 1.212e-012 | -11.855 | -11.917 | -0.062 | |
| Zn(OH)Cl | 1.332e-012 | 1.332e-012 | -11.876 | -11.876 | 0.000 | |
| MnCl3- | 2.301e-014 | 1.995e-014 | -13.638 | -13.700 | -0.062 | |
| ZnCl3- | 1.922e-014 | 1.666e-014 | -13.716 | -13.778 | -0.062 | |
| ZnCl4-2 | 1.779e-016 | 9.991e-017 | -15.750 | -16.000 | -0.251 | |
| FeCl2 | 5.145e-018 | 5.145e-018 | -17.289 | -17.289 | 0.000 | |
| FeCl4- | 7.919e-019 | 6.866e-019 | -18.101 | -18.163 | -0.062 | |
| CuCl2- | 6.289e-020 | 5.452e-020 | -19.201 | -19.263 | -0.062 | |
| CuCl4-2 | 2.428e-021 | 1.363e-021 | -20.615 | -20.865 | -0.251 | |
| CuCl3-2 | 4.934e-022 | 2.770e-022 | -21.307 | -21.557 | -0.251 | |
| FeCl4-2 | 1.657e-023 | 9.306e-024 | -22.781 | -23.031 | -0.251 | |
| Cl (1) | 1.240e-017 | | | | | |
| HClO | 1.240e-017 | 1.240e-017 | -16.907 | -16.907 | 0.000 | |
| ClO- | 7.280e-022 | 6.312e-022 | -21.138 | -21.200 | -0.062 | |
| Cl (3) | 1.243e-032 | | | | | |
| ClO2- | 7.403e-033 | 6.418e-033 | -32.131 | -32.193 | -0.062 | |
| HClO2 | 5.025e-033 | 5.025e-033 | -32.299 | -32.299 | 0.000 | |
| Cl (5) | 5.373e-030 | | | | | |
| ClO3- | 5.373e-030 | 4.644e-030 | -29.270 | -29.333 | -0.063 | |
| Cl (7) | 1.942e-031 | | | | | |
| ClO4- | 1.941e-031 | 1.678e-031 | -30.712 | -30.775 | -0.063 | |
| ZnClO4+ | 1.136e-034 | 9.849e-035 | -33.945 | -34.007 | -0.062 | |
| Cu (1) | 1.580e-018 | | | | | |
| Cu+ | 1.517e-018 | 1.315e-018 | -17.819 | -17.881 | -0.062 | |
| CuCl2- | 6.289e-020 | 5.452e-020 | -19.201 | -19.263 | -0.062 | |
| CuCl3-2 | 4.934e-022 | 2.770e-022 | -21.307 | -21.557 | -0.251 | |
| Cu (2) | 3.233e-004 | | | | | |
| Cu+2 | 2.195e-004 | 1.287e-004 | -3.659 | -3.890 | -0.232 | |
| CuSO4 | 1.034e-004 | 1.034e-004 | -3.985 | -3.985 | 0.000 | |
| CuCl+ | 3.213e-007 | 2.786e-007 | -6.493 | -6.555 | -0.062 | |

| | | | | | | |
|-------|------------|------------|------------|----------|----------|--------|
| | CuOH+ | 1.446e-008 | 1.254e-008 | -7.840 | -7.902 | -0.062 |
| | CuCl2 | 1.161e-010 | 1.161e-010 | -9.935 | -9.935 | 0.000 |
| | CuNO2+ | 7.823e-019 | 6.782e-019 | -18.107 | -18.169 | -0.062 |
| | CuCl4-2 | 2.428e-021 | 1.363e-021 | -20.615 | -20.865 | -0.251 |
| | CuO2-2 | 1.035e-030 | 5.809e-031 | -29.985 | -30.236 | -0.251 |
| | Cu(NO2)2 | 3.492e-034 | 3.492e-034 | -33.457 | -33.457 | 0.000 |
| | CuF+ | 0.000e+000 | 0.000e+000 | -45.910 | -45.972 | -0.062 |
| | CuNH3+2 | 0.000e+000 | 0.000e+000 | -57.053 | -57.298 | -0.246 |
| | Cu(NH3)2+2 | 0.000e+000 | 0.000e+000 | -111.067 | -111.313 | -0.246 |
| | Cu(NH3)3+2 | 0.000e+000 | 0.000e+000 | -165.695 | -165.940 | -0.246 |
| F | 6.582e-006 | | | | | |
| | HAsO3F- | 6.557e-006 | 5.684e-006 | -5.183 | -5.245 | -0.062 |
| | AsO3F-2 | 2.575e-008 | 1.446e-008 | -7.589 | -7.840 | -0.251 |
| | AlF+2 | 0.000e+000 | 0.000e+000 | -40.349 | -40.595 | -0.246 |
| | F- | 0.000e+000 | 0.000e+000 | -43.218 | -43.281 | -0.063 |
| | HF | 0.000e+000 | 0.000e+000 | -43.371 | -43.371 | 0.000 |
| | FeF+2 | 0.000e+000 | 0.000e+000 | -43.826 | -44.072 | -0.246 |
| | CaF+ | 0.000e+000 | 0.000e+000 | -45.437 | -45.499 | -0.062 |
| | MgF+ | 0.000e+000 | 0.000e+000 | -45.464 | -45.526 | -0.062 |
| | MnF+ | 0.000e+000 | 0.000e+000 | -45.852 | -45.914 | -0.062 |
| | CuF+ | 0.000e+000 | 0.000e+000 | -45.910 | -45.972 | -0.062 |
| | ZnF+ | 0.000e+000 | 0.000e+000 | -46.577 | -46.639 | -0.062 |
| | NaF | 0.000e+000 | 0.000e+000 | -47.181 | -47.181 | 0.000 |
| | FeF+ | 0.000e+000 | 0.000e+000 | -50.537 | -50.599 | -0.062 |
| | AlF2+ | 0.000e+000 | 0.000e+000 | -78.214 | -78.276 | -0.062 |
| | FeF2+ | 0.000e+000 | 0.000e+000 | -83.082 | -83.144 | -0.062 |
| | H2F2 | 0.000e+000 | 0.000e+000 | -86.347 | -86.347 | 0.000 |
| | HF2- | 0.000e+000 | 0.000e+000 | -87.206 | -87.268 | -0.062 |
| | AlF3 | 0.000e+000 | 0.000e+000 | -117.458 | -117.458 | 0.000 |
| | AlF4- | 0.000e+000 | 0.000e+000 | -158.277 | -158.339 | -0.062 |
| Fe(2) | 4.756e-009 | | | | | |
| | Fe+2 | 3.586e-009 | 2.103e-009 | -8.445 | -8.677 | -0.232 |
| | FeSO4 | 1.169e-009 | 1.169e-009 | -8.932 | -8.932 | 0.000 |
| | FeCl+ | 1.398e-012 | 1.212e-012 | -11.855 | -11.917 | -0.062 |
| | FeOH+ | 1.448e-015 | 1.255e-015 | -14.839 | -14.901 | -0.062 |
| | FeCl2 | 5.145e-018 | 5.145e-018 | -17.289 | -17.289 | 0.000 |
| | Fe(OH)2 | 1.882e-023 | 1.882e-023 | -22.725 | -22.725 | 0.000 |
| | FeCl4-2 | 1.657e-023 | 9.306e-024 | -22.781 | -23.031 | -0.251 |
| | Fe(OH)3- | 1.632e-030 | 1.415e-030 | -29.787 | -29.849 | -0.062 |
| | Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -41.323 | -41.573 | -0.251 |
| | FeF+ | 0.000e+000 | 0.000e+000 | -50.537 | -50.599 | -0.062 |
| Fe(3) | 3.722e-004 | | | | | |
| | FeOH+2 | 2.319e-004 | 1.317e-004 | -3.635 | -3.880 | -0.246 |
| | Fe(OH)2+ | 9.497e-005 | 8.233e-005 | -4.022 | -4.084 | -0.062 |
| | Fe+3 | 3.188e-005 | 1.080e-005 | -4.497 | -4.966 | -0.470 |
| | FeSO4+ | 4.230e-006 | 3.667e-006 | -5.374 | -5.436 | -0.062 |
| | Fe2(OH)2+4 | 4.138e-006 | 4.669e-007 | -5.383 | -6.331 | -0.948 |
| | Fe(SO4)2- | 2.509e-007 | 2.175e-007 | -6.601 | -6.663 | -0.062 |
| | Fe3(OH)4+5 | 2.282e-007 | 8.031e-009 | -6.642 | -8.095 | -1.453 |
| | Fe(OH)3 | 7.271e-008 | 7.271e-008 | -7.138 | -7.138 | 0.000 |
| | FeNO3+2 | 1.686e-008 | 9.575e-009 | -7.773 | -8.019 | -0.246 |
| | FeCl+2 | 2.508e-009 | 1.424e-009 | -8.601 | -8.846 | -0.246 |
| | FeCl2+ | 1.052e-009 | 9.123e-010 | -8.978 | -9.040 | -0.062 |
| | Fe(OH)4- | 3.977e-014 | 3.448e-014 | -13.400 | -13.462 | -0.062 |
| | FeNO2+2 | 1.352e-018 | 7.679e-019 | -17.869 | -18.115 | -0.246 |
| | FeCl4- | 7.919e-019 | 6.866e-019 | -18.101 | -18.163 | -0.062 |
| | FeF+2 | 0.000e+000 | 0.000e+000 | -43.826 | -44.072 | -0.246 |
| | FeF2+ | 0.000e+000 | 0.000e+000 | -83.082 | -83.144 | -0.062 |
| H(0) | 0.000e+000 | | | | | |
| | H2 | 0.000e+000 | 0.000e+000 | -43.113 | -43.111 | 0.002 |
| K | 4.877e-004 | | | | | |
| | K+ | 4.744e-004 | 4.088e-004 | -3.324 | -3.389 | -0.065 |
| | KSO4- | 1.335e-005 | 1.157e-005 | -4.875 | -4.937 | -0.062 |
| | KCl | 1.086e-008 | 1.086e-008 | -7.964 | -7.964 | 0.000 |
| | KHSO4 | 5.408e-009 | 5.408e-009 | -8.267 | -8.267 | 0.000 |
| | KOH | 2.676e-015 | 2.676e-015 | -14.573 | -14.573 | 0.000 |
| Mg | 6.093e-004 | | | | | |

| | | | | | |
|------------|------------|------------|----------|----------|--------|
| Mg+2 | 3.879e-004 | 2.361e-004 | -3.411 | -3.627 | -0.216 |
| MgSO4 | 2.212e-004 | 2.212e-004 | -3.655 | -3.655 | 0.000 |
| MgCl+ | 1.682e-007 | 1.458e-007 | -6.774 | -6.836 | -0.062 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -40.206 | -41.153 | -0.948 |
| MgF+ | 0.000e+000 | 0.000e+000 | -45.464 | -45.526 | -0.062 |
| Mn(2) | 2.228e-004 | | | | |
| Mn+2 | 1.477e-004 | 8.659e-005 | -3.831 | -4.063 | -0.232 |
| MnSO4 | 7.495e-005 | 7.495e-005 | -4.125 | -4.125 | 0.000 |
| MnCl+ | 1.683e-007 | 1.459e-007 | -6.774 | -6.836 | -0.062 |
| MnNO3+ | 1.403e-008 | 1.216e-008 | -7.853 | -7.915 | -0.062 |
| MnOH+ | 4.847e-012 | 4.202e-012 | -11.315 | -11.377 | -0.062 |
| Mn(NO3)2 | 2.707e-012 | 2.707e-012 | -11.567 | -11.567 | 0.000 |
| MnCl3- | 2.301e-014 | 1.995e-014 | -13.638 | -13.700 | -0.062 |
| Mn2OH+3 | 1.361e-015 | 3.899e-016 | -14.866 | -15.409 | -0.543 |
| Mn(OH)2 | 1.947e-020 | 1.947e-020 | -19.711 | -19.711 | 0.000 |
| Mn2(OH)3+ | 7.327e-023 | 6.352e-023 | -22.135 | -22.197 | -0.062 |
| Mn(OH)3- | 3.978e-029 | 3.449e-029 | -28.400 | -28.462 | -0.062 |
| Mn(OH)4-2 | 9.819e-040 | 5.514e-040 | -39.008 | -39.259 | -0.251 |
| MnF+ | 0.000e+000 | 0.000e+000 | -45.852 | -45.914 | -0.062 |
| Mn(3) | 4.322e-013 | | | | |
| Mn+3 | 4.322e-013 | 1.238e-013 | -12.364 | -12.907 | -0.543 |
| Mn(6) | 7.347e-030 | | | | |
| MnO4-2 | 7.347e-030 | 4.126e-030 | -29.134 | -29.385 | -0.251 |
| Mn(7) | 1.126e-022 | | | | |
| MnO4- | 1.126e-022 | 9.737e-023 | -21.948 | -22.012 | -0.063 |
| N(-03) | 0.000e+000 | | | | |
| HN3 | 0.000e+000 | 0.000e+000 | -82.644 | -82.644 | 0.000 |
| N3- | 0.000e+000 | 0.000e+000 | -84.008 | -84.070 | -0.062 |
| ZnN3+ | 0.000e+000 | 0.000e+000 | -88.074 | -88.136 | -0.062 |
| Zn(N3)2 | 0.000e+000 | 0.000e+000 | -171.452 | -171.452 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH4+ | 0.000e+000 | 0.000e+000 | -51.418 | -51.484 | -0.066 |
| CuNH3+2 | 0.000e+000 | 0.000e+000 | -57.053 | -57.298 | -0.246 |
| NH3 | 0.000e+000 | 0.000e+000 | -57.448 | -57.448 | 0.000 |
| Zn(NH3)+2 | 0.000e+000 | 0.000e+000 | -59.658 | -59.903 | -0.246 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -62.177 | -62.239 | -0.062 |
| Cu(NH3)2+2 | 0.000e+000 | 0.000e+000 | -111.067 | -111.313 | -0.246 |
| Zn(NH3)2+2 | 0.000e+000 | 0.000e+000 | -114.900 | -115.145 | -0.246 |
| Cu(NH3)3+2 | 0.000e+000 | 0.000e+000 | -165.695 | -165.940 | -0.246 |
| Zn(NH3)3+2 | 0.000e+000 | 0.000e+000 | -170.141 | -170.387 | -0.246 |
| Zn(NH3)4+2 | 0.000e+000 | 0.000e+000 | -225.657 | -225.902 | -0.246 |
| N(0) | 7.987e-008 | | | | |
| N2 | 3.993e-008 | 3.993e-008 | -7.399 | -7.399 | 0.000 |
| N(3) | 1.060e-016 | | | | |
| NO2- | 5.839e-017 | 5.031e-017 | -16.234 | -16.298 | -0.065 |
| HNO2 | 4.547e-017 | 4.547e-017 | -16.342 | -16.342 | 0.000 |
| FeNO2+2 | 1.352e-018 | 7.679e-019 | -17.869 | -18.115 | -0.246 |
| CuNO2+ | 7.823e-019 | 6.782e-019 | -18.107 | -18.169 | -0.062 |
| Cu(NO2)2 | 3.492e-034 | 3.492e-034 | -33.457 | -33.457 | 0.000 |
| N(5) | 1.035e-004 | | | | |
| NO3- | 1.028e-004 | 8.862e-005 | -3.988 | -4.052 | -0.065 |
| CaNO3+ | 6.103e-007 | 5.292e-007 | -6.214 | -6.276 | -0.062 |
| FeNO3+2 | 1.686e-008 | 9.575e-009 | -7.773 | -8.019 | -0.246 |
| MnNO3+ | 1.403e-008 | 1.216e-008 | -7.853 | -7.915 | -0.062 |
| HNO3 | 2.454e-009 | 2.454e-009 | -8.610 | -8.610 | 0.000 |
| Mn(NO3)2 | 2.707e-012 | 2.707e-012 | -11.567 | -11.567 | 0.000 |
| Na | 1.391e-003 | | | | |
| Na+ | 1.359e-003 | 1.178e-003 | -2.867 | -2.929 | -0.062 |
| NaSO4- | 3.150e-005 | 2.731e-005 | -4.502 | -4.564 | -0.062 |
| NaCl | 1.639e-007 | 1.639e-007 | -6.786 | -6.786 | 0.000 |
| NaOH | 3.698e-015 | 3.698e-015 | -14.432 | -14.432 | 0.000 |
| NaAlO2 | 1.800e-018 | 1.800e-018 | -17.745 | -17.745 | 0.000 |
| NaF | 0.000e+000 | 0.000e+000 | -47.181 | -47.181 | 0.000 |
| O(0) | 2.111e-006 | | | | |
| O2 | 1.055e-006 | 1.061e-006 | -5.977 | -5.974 | 0.002 |
| S(-2) | 0.000e+000 | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -128.332 | -128.332 | 0.000 |

| | | | | | |
|------------|------------|------------|----------|----------|--------|
| HS- | 0.000e+000 | 0.000e+000 | -132.002 | -132.065 | -0.063 |
| S-2 | 0.000e+000 | 0.000e+000 | -141.474 | -141.715 | -0.241 |
| S2-2 | 0.000e+000 | 0.000e+000 | -233.609 | -233.859 | -0.251 |
| HAsS2 | 0.000e+000 | 0.000e+000 | -275.826 | -275.826 | 0.000 |
| S3-2 | 0.000e+000 | 0.000e+000 | -325.795 | -326.045 | -0.251 |
| S4-2 | 0.000e+000 | 0.000e+000 | -418.208 | -418.458 | -0.251 |
| S5-2 | 0.000e+000 | 0.000e+000 | -510.837 | -511.088 | -0.251 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -132.736 | -132.987 | -0.251 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -135.187 | -135.249 | -0.062 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -120.662 | -120.902 | -0.241 |
| S(4) | 0.000e+000 | | | | |
| HSO3- | 0.000e+000 | 0.000e+000 | -42.068 | -42.130 | -0.062 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -43.425 | -43.425 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -43.525 | -43.525 | 0.000 |
| SO3-2 | 0.000e+000 | 0.000e+000 | -45.840 | -46.086 | -0.246 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -59.593 | -59.843 | -0.251 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -154.261 | -154.512 | -0.251 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -233.024 | -233.275 | -0.251 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -340.667 | -340.918 | -0.251 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -88.840 | -89.090 | -0.251 |
| S(6) | 7.857e-003 | | | | |
| SO4-2 | 6.247e-003 | 3.508e-003 | -2.204 | -2.455 | -0.251 |
| CaSO4 | 6.105e-004 | 6.105e-004 | -3.214 | -3.214 | 0.000 |
| MgSO4 | 2.212e-004 | 2.212e-004 | -3.655 | -3.655 | 0.000 |
| HSO4- | 2.164e-004 | 1.876e-004 | -3.665 | -3.727 | -0.062 |
| AlSO4+ | 2.011e-004 | 1.743e-004 | -3.697 | -3.759 | -0.062 |
| CuSO4 | 1.034e-004 | 1.034e-004 | -3.985 | -3.985 | 0.000 |
| MnSO4 | 7.495e-005 | 7.495e-005 | -4.125 | -4.125 | 0.000 |
| Al(SO4)2- | 5.476e-005 | 4.747e-005 | -4.262 | -4.324 | -0.062 |
| NaSO4- | 3.150e-005 | 2.731e-005 | -4.502 | -4.564 | -0.062 |
| ZnSO4 | 2.288e-005 | 2.288e-005 | -4.641 | -4.641 | 0.000 |
| KSO4- | 1.335e-005 | 1.157e-005 | -4.875 | -4.937 | -0.062 |
| FeSO4+ | 4.230e-006 | 3.667e-006 | -5.374 | -5.436 | -0.062 |
| Fe(SO4)2- | 2.509e-007 | 2.175e-007 | -6.601 | -6.663 | -0.062 |
| KHSO4 | 5.408e-009 | 5.408e-009 | -8.267 | -8.267 | 0.000 |
| FeSO4 | 1.169e-009 | 1.169e-009 | -8.932 | -8.932 | 0.000 |
| H2SO4 | 9.375e-011 | 9.375e-011 | -10.028 | -10.028 | 0.000 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -62.177 | -62.239 | -0.062 |
| S(7) | 4.441e-037 | | | | |
| S2O8-2 | 2.220e-037 | 1.247e-037 | -36.654 | -36.904 | -0.251 |
| S(8) | 1.211e-026 | | | | |
| HSO5- | 1.211e-026 | 1.050e-026 | -25.917 | -25.979 | -0.062 |
| Zn | 7.586e-005 | | | | |
| Zn+2 | 5.293e-005 | 3.104e-005 | -4.276 | -4.508 | -0.232 |
| ZnSO4 | 2.288e-005 | 2.288e-005 | -4.641 | -4.641 | 0.000 |
| ZnCl+ | 4.759e-008 | 4.126e-008 | -7.322 | -7.384 | -0.062 |
| ZnOH+ | 7.413e-011 | 6.427e-011 | -10.130 | -10.192 | -0.062 |
| ZnCl2 | 3.813e-011 | 3.813e-011 | -10.419 | -10.419 | 0.000 |
| Zn(OH)Cl | 1.332e-012 | 1.332e-012 | -11.876 | -11.876 | 0.000 |
| ZnCl3- | 1.922e-014 | 1.666e-014 | -13.716 | -13.778 | -0.062 |
| Zn(OH)2 | 5.196e-016 | 5.196e-016 | -15.284 | -15.284 | 0.000 |
| ZnCl4-2 | 1.779e-016 | 9.991e-017 | -15.750 | -16.000 | -0.251 |
| Zn(OH)3- | 3.507e-024 | 3.041e-024 | -23.455 | -23.517 | -0.062 |
| Zn(OH)4-2 | 1.743e-033 | 9.787e-034 | -32.759 | -33.009 | -0.251 |
| ZnClO4+ | 1.136e-034 | 9.849e-035 | -33.945 | -34.007 | -0.062 |
| ZnF+ | 0.000e+000 | 0.000e+000 | -46.577 | -46.639 | -0.062 |
| Zn(NH3)+2 | 0.000e+000 | 0.000e+000 | -59.658 | -59.903 | -0.246 |
| ZnN3+ | 0.000e+000 | 0.000e+000 | -88.074 | -88.136 | -0.062 |
| Zn(NH3)2+2 | 0.000e+000 | 0.000e+000 | -114.900 | -115.145 | -0.246 |
| Zn(NH3)3+2 | 0.000e+000 | 0.000e+000 | -170.141 | -170.387 | -0.246 |
| Zn(N3)2 | 0.000e+000 | 0.000e+000 | -171.452 | -171.452 | 0.000 |
| Zn(NH3)4+2 | 0.000e+000 | 0.000e+000 | -225.657 | -225.902 | -0.246 |

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

| Phase | SI | log IAP | log KT | |
|--------------------|---------|---------|---------|--------------------------|
| Al | -139.92 | 10.00 | 149.91 | Al |
| Al(g) | -190.62 | 10.00 | 200.62 | Al |
| Al2(SO4)3 | -34.89 | -15.99 | 18.90 | Al2(SO4)3 |
| Al2(SO4)3:6H2O | -17.55 | -15.99 | 1.56 | Al2(SO4)3:6H2O |
| Alabandite | -132.43 | -132.85 | -0.42 | MnS |
| AlF3 | -116.89 | -134.16 | -17.27 | AlF3 |
| Alum-K | -7.64 | -12.61 | -4.97 | KAl(SO4)2:12H2O |
| Alunite | -1.11 | -1.58 | -0.47 | KAl3(OH)6(SO4)2 |
| Anhydrite | -1.03 | -5.38 | -4.35 | CaSO4 |
| Antarcticite | -13.22 | -9.13 | 4.09 | CaCl2:6H2O |
| Antlerite | -9.75 | -1.02 | 8.73 | Cu3(SO4)(OH)4 |
| Aphthitalite | -14.12 | -18.00 | -3.89 | NaK3(SO4)2 |
| Arcanite | -7.39 | -9.23 | -1.84 | K2SO4 |
| Arsenolite | -51.41 | -71.25 | -19.84 | As2O3 |
| Arsenopyrite | -216.50 | -230.94 | -14.45 | FeAsS |
| As | -73.83 | -31.14 | 42.68 | As |
| As2O5 | -18.29 | -16.16 | 2.14 | As2O5 |
| As4O6(cubi) | -102.67 | -142.50 | -39.82 | As4O6 |
| As4O6(mono) | -102.45 | -142.50 | -40.05 | As4O6 |
| Atacamite | -16.37 | -2.11 | 14.26 | Cu4Cl2(OH)6 |
| Bassanite | -1.67 | -5.38 | -3.71 | CaSO4:0.5H2O |
| Birnessite | -9.82 | -95.36 | -85.55 | Mn8O14:5H2O |
| Bischofite | -14.22 | -9.83 | 4.39 | MgCl2:6H2O |
| Bixbyite | -5.19 | -6.16 | -0.96 | Mn2O3 |
| Bloedite | -11.92 | -14.39 | -2.48 | Na2Mg(SO4)2:4H2O |
| Boehmite | -2.04 | 5.51 | 7.55 | AlO2H |
| Bornite | -496.71 | -599.25 | -102.53 | Cu5FeS4 |
| Brochantite | -13.78 | 1.64 | 15.42 | Cu4(SO4)(OH)6 |
| Brucite | -13.36 | 2.93 | 16.28 | Mg(OH)2 |
| Ca | -133.22 | 6.62 | 139.83 | Ca |
| Ca(g) | -158.46 | 6.62 | 165.07 | Ca |
| Ca2Al2O5:8H2O | -41.28 | 18.28 | 59.57 | Ca2Al2O5:8H2O |
| Ca2Cl2(OH)2:H2O | -31.79 | -5.50 | 26.29 | Ca2Cl2(OH)2:H2O |
| Ca3(AsO4)2 | -23.08 | -5.27 | 17.80 | Ca3(AsO4)2 |
| Ca3Al2O6 | -91.12 | 21.91 | 113.03 | Ca3Al2O6 |
| Ca4Al2Fe2O10 | -105.22 | 35.26 | 140.48 | Ca4Al2Fe2O10 |
| Ca4Al2O7:13H2O | -81.71 | 25.54 | 107.25 | Ca4Al2O7:13H2O |
| Ca4Al2O7:19H2O | -78.14 | 25.54 | 103.68 | Ca4Al2O7:19H2O |
| Ca4Cl2(OH)6:13H2O | -66.57 | 1.76 | 68.33 | Ca4Cl2(OH)6:13H2O |
| CaAl2O4 | -32.25 | 14.66 | 46.91 | CaAl2O4 |
| CaAl2O4:10H2O | -23.34 | 14.66 | 37.99 | CaAl2O4:10H2O |
| CaAl4O7 | -42.91 | 25.69 | 68.59 | CaAl4O7 |
| Carnallite | -20.59 | -16.32 | 4.27 | KMgCl3:6H2O |
| CaSO4:0.5H2O(beta) | -1.84 | -5.38 | -3.54 | CaSO4:0.5H2O |
| Chalcanthite | -3.72 | -6.35 | -2.63 | CuSO4:5H2O |
| Chalcocite | -129.81 | -164.55 | -34.74 | Cu2S |
| Chalcocyanite | -9.26 | -6.35 | 2.91 | CuSO4 |
| Chalcopyrite | -237.54 | -270.15 | -32.60 | CuFeS2 |
| Chloromagnesite | -31.65 | -9.83 | 21.82 | MgCl2 |
| Cl2(g) | -18.74 | -15.74 | 2.99 | Cl2 |
| Claudetite | -51.45 | -71.25 | -19.80 | As2O3 |
| Corundum | -7.26 | 11.03 | 18.29 | Al2O3 |
| Covellite | -109.82 | -132.68 | -22.86 | CuS |
| Cu | -25.85 | 5.65 | 31.50 | Cu |
| Cu(g) | -78.01 | 5.65 | 83.66 | Cu |
| CuCl2 | -13.82 | -10.09 | 3.72 | CuCl2 |
| CuF | -68.24 | -61.16 | 7.08 | CuF |
| CuF2 | -89.83 | -90.45 | -0.62 | CuF2 |
| CuF2:2H2O | -85.90 | -90.45 | -4.55 | CuF2:2H2O |
| Cuprite | -27.30 | -29.21 | -1.91 | Cu2O |
| Delafoosite | -3.31 | -9.74 | -6.44 | CuFeO2 |
| Diaspore | -1.63 | 5.51 | 7.15 | AlHO2 |
| Epsomite | -4.12 | -6.08 | -1.96 | MgSO4:7H2O |
| Ettringite | -56.69 | 5.77 | 62.46 | Ca6Al2(SO4)3(OH)12:26H2O |

| | | | | |
|-------------------------|---------|---------|--------|-------------------------|
| F2(g) | -151.81 | -96.10 | 55.71 | F2 |
| Fe | -58.16 | 0.86 | 59.02 | Fe |
| Fe(OH)2 | -16.02 | -2.13 | 13.89 | Fe(OH)2 |
| Fe(OH)3 | -0.78 | 4.86 | 5.64 | Fe(OH)3 |
| Fe2(SO4)3 | -20.34 | -17.30 | 3.05 | Fe2(SO4)3 |
| FeF2 | -92.82 | -95.24 | -2.42 | FeF2 |
| FeF3 | -115.55 | -134.81 | -19.26 | FeF3 |
| FeO | -15.65 | -2.13 | 13.52 | FeO |
| Ferrite-Ca | -8.14 | 13.35 | 21.50 | CaFe2O4 |
| Ferrite-Cu | 2.10 | 12.39 | 10.28 | CuFe2O4 |
| Ferrite-Dicalcium | -39.82 | 16.98 | 56.80 | Ca2Fe2O5 |
| Ferrite-Mg | -8.37 | 12.65 | 21.02 | MgFe2O4 |
| Ferrite-Zn | 0.07 | 11.77 | 11.70 | ZnFe2O4 |
| FeSO4 | -13.74 | -11.13 | 2.61 | FeSO4 |
| Fluorite | -79.42 | -89.49 | -10.07 | CaF2 |
| Gibbsite | -2.23 | 5.51 | 7.74 | Al(OH)3 |
| Glauberite | -8.22 | -13.69 | -5.47 | Na2Ca(SO4)2 |
| Goethite | 4.33 | 4.86 | 0.53 | FeOOH |
| Gypsum | -0.85 | -5.38 | -4.53 | CaSO4:2H2O |
| H2(g) | -40.01 | -43.11 | -3.10 | H2 |
| H2O(g) | -1.59 | -0.00 | 1.59 | H2O |
| H2S(g) | -127.35 | -135.34 | -7.99 | H2S |
| Halite | -7.59 | -6.03 | 1.56 | NaCl |
| Hausmannite | -13.81 | -3.67 | 10.14 | Mn3O4 |
| HCl(g) | -12.68 | -6.38 | 6.30 | HCl |
| Hematite | 9.65 | 9.72 | 0.08 | Fe2O3 |
| Hercynite | -19.90 | 8.90 | 28.80 | FeAl2O4 |
| Hexahydrite | -4.36 | -6.08 | -1.73 | MgSO4:6H2O |
| Hydrophilite | -20.87 | -9.13 | 11.75 | CaCl2 |
| Ice | -0.14 | -0.00 | 0.14 | H2O |
| Jarosite | 5.87 | -3.54 | -9.41 | KFe3(SO4)2(OH)6 |
| Jarosite-Na | 2.37 | -3.08 | -5.45 | NaFe3(SO4)2(OH)6 |
| K | -69.60 | 1.38 | 70.98 | K |
| K(g) | -80.20 | 1.38 | 81.58 | K |
| K2O | -84.26 | -0.22 | 84.04 | K2O |
| K3H(SO4)2 | -14.73 | -18.35 | -3.62 | K3H(SO4)2 |
| Kainite | -12.26 | -12.57 | -0.31 | KMgClSO4:3H2O |
| KAl(SO4)2 | -15.88 | -12.61 | 3.27 | KAl(SO4)2 |
| Katoite | -57.03 | 21.91 | 78.94 | Ca3Al2H12O12 |
| Kieserite | -5.81 | -6.08 | -0.27 | MgSO4:H2O |
| KMgCl3 | -37.57 | -16.32 | 21.25 | KMgCl3 |
| KMgCl3:2H2O | -30.28 | -16.32 | 13.96 | KMgCl3:2H2O |
| Lammerite | -9.73 | -8.17 | 1.55 | Cu3(AsO4)2 |
| Lawrencite | -23.94 | -14.88 | 9.05 | FeCl2 |
| Leonite | -11.20 | -15.31 | -4.11 | K2Mg(SO4)2:4H2O |
| Lime | -28.94 | 3.63 | 32.57 | CaO |
| Magnetite | -2.82 | 7.60 | 10.42 | Fe3O4 |
| Manganite | -2.91 | -3.08 | -0.16 | MnO(OH) |
| Manganosite | -15.43 | 2.49 | 17.92 | MnO |
| Mayenite | -373.41 | 120.74 | 494.15 | Ca12Al14O33 |
| Melanterite | -8.73 | -11.13 | -2.40 | FeSO4:7H2O |
| Mercallite | -7.68 | -9.12 | -1.44 | KHSO4 |
| Mg | -116.61 | 5.91 | 122.52 | Mg |
| Mg(g) | -136.33 | 5.91 | 142.25 | Mg |
| Mg1.25SO4(OH)0.5:0.5H2O | -10.55 | -5.35 | 5.20 | Mg1.25SO4(OH)0.5:0.5H2O |
| Mg1.5SO4(OH) | -13.83 | -4.62 | 9.21 | Mg1.5SO4(OH) |
| MgCl2:2H2O | -22.56 | -9.83 | 12.73 | MgCl2:2H2O |
| MgCl2:4H2O | -17.13 | -9.83 | 7.30 | MgCl2:4H2O |
| MgCl2:H2O | -25.90 | -9.83 | 16.07 | MgCl2:H2O |
| MgOHCl | -19.34 | -3.45 | 15.89 | MgOHCl |
| MgSO4 | -10.91 | -6.08 | 4.83 | MgSO4 |
| Mirabilite | -7.16 | -8.31 | -1.15 | Na2SO4:10H2O |
| Misenite | -52.87 | -63.95 | -11.08 | K8H6(SO4)7 |
| Mn | -77.46 | 5.48 | 82.93 | Mn |
| Mn(OH)2(am) | -12.82 | 2.49 | 15.31 | Mn(OH)2 |
| Mn(OH)3 | -9.42 | -3.08 | 6.34 | Mn(OH)3 |
| MnCl2:2H2O | -14.26 | -10.27 | 4.00 | MnCl2:2H2O |

| | | | | |
|------------------|---------|---------|--------|--------------------|
| MnCl2:4H2O | -13.02 | -10.27 | 2.75 | MnCl2:4H2O |
| MnCl2:H2O | -15.81 | -10.27 | 5.54 | MnCl2:H2O |
| MnO2 (gamma) | -0.60 | -16.72 | -16.13 | MnO2 |
| MnSO4 | -9.13 | -6.52 | 2.61 | MnSO4 |
| Molysite | -27.74 | -14.27 | 13.47 | FeCl3 |
| N2(g) | -4.22 | -7.40 | -3.18 | N2 |
| Na | -65.53 | 1.84 | 67.37 | Na |
| Na(g) | -79.02 | 1.84 | 80.86 | Na |
| Na2O | -66.72 | 0.69 | 67.42 | Na2O |
| Na3H(SO4)2 | -16.08 | -16.97 | -0.89 | Na3H(SO4)2 |
| Na4Ca(SO4)3:2H2O | -16.11 | -22.00 | -5.89 | Na4Ca(SO4)3:2H2O |
| NaFeO2 | -14.67 | 5.21 | 19.88 | NaFeO2 |
| Nantokite | -14.22 | -20.98 | -6.77 | CuCl |
| NH3(g) | -59.24 | -57.45 | 1.80 | NH3 |
| Niter | -7.22 | -7.44 | -0.22 | KNO3 |
| NO(g) | -18.82 | -18.08 | 0.74 | NO |
| NO2(g) | -14.18 | -5.83 | 8.35 | NO2 |
| O2(g) | -3.08 | -5.97 | -2.89 | O2 |
| Orpiment | -397.79 | -477.27 | -79.49 | As2S3 |
| Oxychloride-Mg | -26.36 | -0.53 | 25.83 | Mg2Cl(OH)3:4H2O |
| Pentahydrate | -4.70 | -6.08 | -1.39 | MgSO4:5H2O |
| Periclase | -18.40 | 2.93 | 21.33 | MgO |
| Picromerite | -10.87 | -15.31 | -4.44 | K2Mg(SO4)2:6H2O |
| Polyhalite | -11.76 | -26.07 | -14.31 | K2MgCa2(SO4)4:2H2O |
| Portlandite | -18.92 | 3.63 | 22.55 | Ca(OH)2 |
| Pyrite | -216.52 | -241.22 | -24.70 | FeS2 |
| Pyrolusite | 0.94 | -16.72 | -17.66 | MnO2 |
| Pyrrhotite | -133.73 | -137.47 | -3.74 | FeS |
| Realgar | -154.78 | -215.06 | -60.28 | AsS |
| S | -93.22 | -138.33 | -45.11 | S |
| S2(g) | -200.33 | -207.51 | -7.19 | S2 |
| Scacchite | -19.01 | -10.27 | 8.74 | MnCl2 |
| Sellaite | -80.75 | -90.19 | -9.44 | MgF2 |
| SO2(g) | -43.70 | -43.52 | 0.18 | SO2 |
| Sphalerite | -121.83 | -133.30 | -11.47 | ZnS |
| Spinel | -23.65 | 13.95 | 37.61 | Al2MgO4 |
| Starkeyite | -5.08 | -6.08 | -1.00 | MgSO4:4H2O |
| Sylvite | -7.32 | -6.49 | 0.83 | KCl |
| Syngenite | -7.01 | -14.61 | -7.60 | K2Ca(SO4)2:H2O |
| Tachyhydrite | -45.93 | -28.79 | 17.14 | Mg2CaCl6:12H2O |
| Tenorite | -4.99 | 2.66 | 7.65 | CuO |
| Thenardite | -7.95 | -8.31 | -0.36 | Na2SO4 |
| Todorokite | -8.59 | -54.41 | -45.82 | Mn7O12:3H2O |
| Troilite | -133.62 | -137.47 | -3.84 | FeS |
| Wurtzite | -124.13 | -133.30 | -9.17 | ZnS |
| Wustite | -13.67 | -1.27 | 12.40 | Fe.947O |
| Zincite | -9.16 | 2.04 | 11.20 | ZnO |
| Zn | -63.76 | 5.03 | 68.79 | Zn |
| Zn(ClO4)2:6H2O | -71.69 | -66.06 | 5.63 | Zn(ClO4)2:6H2O |
| Zn(g) | -80.38 | 5.03 | 85.41 | Zn |
| Zn(NO3)2:6H2O | -16.01 | -12.61 | 3.40 | Zn(NO3)2:6H2O |
| Zn(OH)2(beta) | -9.89 | 2.04 | 11.93 | Zn(OH)2 |
| Zn(OH)2(epsilon) | -9.62 | 2.04 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -9.84 | 2.04 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -17.58 | -2.29 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -12.50 | -4.92 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -19.34 | -10.03 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -30.97 | -11.88 | 19.09 | Zn3O(SO4)2 |
| Zn5(NO3)2(OH)8 | -47.10 | -4.44 | 42.67 | Zn5(NO3)2(OH)8 |
| ZnCl2 | -17.79 | -10.71 | 7.08 | ZnCl2 |
| ZnCl2(NH3)2 | -118.60 | -125.61 | -7.01 | ZnCl2(NH3)2 |
| ZnCl2(NH3)4 | -233.80 | -240.50 | -6.71 | ZnCl2(NH3)4 |
| ZnCl2(NH3)6 | -350.66 | -355.40 | -4.74 | ZnCl2(NH3)6 |
| ZnF2 | -90.58 | -91.07 | -0.49 | ZnF2 |
| ZnSO4 | -10.50 | -6.96 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -5.26 | -6.96 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -5.09 | -6.96 | -1.88 | ZnSO4:7H2O |

ZnSO4:H2O -6.41 -6.96 -0.55 ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
