
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 4
temp 25
pH 3.17
pe 12
redox pe
units mg/l
density 1
Cl 46.9
S(6) 1089.6
Al 25.6
As 5.0
Ca 201.4
Cu 35.1
Fe 170.2
K 69.2
Mg 19.8
Mn 20.6
Na 33.2
Zn 17.4
C(4) 0
water 1 # kg
SOLUTION 3 AS2
temp 25
units mg/l
pe 10
pH 6.98
Cl 678.5
S(6) 427.00
Al 0.00
As 0.1526
Ca 238.3
Cu 0.00
Fe 0.00
K 40.73
Mg 13.69
Mn 0.114
Na 392.9
Zn 2.44
C(4) 153.72
MIX 2
1 1

```

3      1
SELECTED_OUTPUT
file          DAM_AS2
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 4

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

| Elements | Molality | Moles |
|----------|------------|------------|
| Al | 9.504e-004 | 9.504e-004 |
| As | 6.685e-005 | 6.685e-005 |
| Ca | 5.034e-003 | 5.034e-003 |
| Cl | 1.325e-003 | 1.325e-003 |
| Cu | 5.533e-004 | 5.533e-004 |
| Fe | 3.053e-003 | 3.053e-003 |
| K | 1.773e-003 | 1.773e-003 |
| Mg | 8.161e-004 | 8.161e-004 |
| Mn | 3.756e-004 | 3.756e-004 |
| Na | 1.447e-003 | 1.447e-003 |
| S(6) | 1.136e-002 | 1.136e-002 |
| Zn | 2.666e-004 | 2.666e-004 |

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

```

pH = 3.170
pe = 12.000
Activity of water = 1.000
Ionic strength = 3.718e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -2.718e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = 3.154e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 8.05
Iterations = 8
Total H = 1.110537e+002
Total O = 5.557286e+001

```

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|----------------|------------|------------|-----------------|-----------------|--------------|
| H+ | 7.785e-004 | 6.761e-004 | -3.109 | -3.170 | -0.061 |
| OH- | 1.709e-011 | 1.424e-011 | -10.767 | -10.846 | -0.079 |
| H2O | 5.553e+001 | 9.996e-001 | 1.744 | -0.000 | 0.000 |
| Al | 9.504e-004 | | | | |
| AlSO4+ | 4.577e-004 | 3.832e-004 | -3.339 | -3.417 | -0.077 |
| Al+3 | 3.507e-004 | 9.580e-005 | -3.455 | -4.019 | -0.564 |
| Al(SO4)2- | 1.389e-004 | 1.163e-004 | -3.857 | -3.935 | -0.077 |
| AlOH+2 | 3.206e-006 | 1.587e-006 | -5.494 | -5.799 | -0.305 |
| Al(OH)2+ | 6.507e-009 | 5.448e-009 | -8.187 | -8.264 | -0.077 |
| Al2(OH)2+4 | 6.033e-009 | 4.095e-010 | -8.219 | -9.388 | -1.168 |
| HALO2 | 1.173e-011 | 1.173e-011 | -10.931 | -10.931 | 0.000 |
| Al3(OH)4+5 | 3.369e-012 | 5.535e-014 | -11.472 | -13.257 | -1.784 |
| AlO2- | 7.097e-015 | 5.942e-015 | -14.149 | -14.226 | -0.077 |
| NaAlO2 | 1.338e-018 | 1.338e-018 | -17.874 | -17.874 | 0.000 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -46.038 | -49.537 | -3.499 |

| | | | | | | |
|----------|------------|------------|----------|----------|--------|--|
| As(-3) | 0.000e+000 | | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -112.033 | -112.033 | 0.000 | |
| As(3) | 1.610e-016 | | | | | |
| HAsO2 | 8.593e-017 | 8.593e-017 | -16.066 | -16.066 | 0.000 | |
| As(OH)3 | 7.510e-017 | 7.510e-017 | -16.124 | -16.124 | 0.000 | |
| H2AsO3- | 8.114e-023 | 6.793e-023 | -22.091 | -22.168 | -0.077 | |
| AsO2- | 7.760e-023 | 6.497e-023 | -22.110 | -22.187 | -0.077 | |
| AsO2OH-2 | 2.019e-030 | 9.817e-031 | -29.695 | -30.008 | -0.313 | |
| As(5) | 6.685e-005 | | | | | |
| H2AsO4- | 6.077e-005 | 5.088e-005 | -4.216 | -4.293 | -0.077 | |
| H3AsO4 | 6.059e-006 | 6.059e-006 | -5.218 | -5.218 | 0.000 | |
| HAsO4-2 | 2.569e-008 | 1.249e-008 | -7.590 | -7.903 | -0.313 | |
| AsO4-3 | 2.411e-016 | 4.740e-017 | -15.618 | -16.324 | -0.706 | |
| Ca | 5.034e-003 | | | | | |
| Ca+2 | 3.882e-003 | 2.017e-003 | -2.411 | -2.695 | -0.284 | |
| CaSO4 | 1.152e-003 | 1.152e-003 | -2.939 | -2.939 | 0.000 | |
| CaCl+ | 5.599e-007 | 4.688e-007 | -6.252 | -6.329 | -0.077 | |
| CaCl2 | 6.044e-010 | 6.044e-010 | -9.219 | -9.219 | 0.000 | |
| CaOH+ | 5.032e-013 | 4.213e-013 | -12.298 | -12.375 | -0.077 | |
| Cl(-1) | 1.325e-003 | | | | | |
| Cl- | 1.322e-003 | 1.096e-003 | -2.879 | -2.960 | -0.081 | |
| CuCl+ | 7.019e-007 | 5.877e-007 | -6.154 | -6.231 | -0.077 | |
| CaCl+ | 5.599e-007 | 4.688e-007 | -6.252 | -6.329 | -0.077 | |
| FeCl+ | 5.035e-007 | 4.215e-007 | -6.298 | -6.375 | -0.077 | |
| MnCl+ | 3.622e-007 | 3.033e-007 | -6.441 | -6.518 | -0.077 | |
| MgCl+ | 2.911e-007 | 2.438e-007 | -6.536 | -6.613 | -0.077 | |
| NaCl | 2.275e-007 | 2.275e-007 | -6.643 | -6.643 | 0.000 | |
| ZnCl+ | 2.134e-007 | 1.787e-007 | -6.671 | -6.748 | -0.077 | |
| HCl | 1.665e-007 | 1.665e-007 | -6.779 | -6.779 | 0.000 | |
| KCl | 5.248e-008 | 5.248e-008 | -7.280 | -7.280 | 0.000 | |
| FeCl+2 | 1.867e-008 | 9.244e-009 | -7.729 | -8.034 | -0.305 | |
| FeCl2+ | 9.799e-009 | 8.204e-009 | -8.009 | -8.086 | -0.077 | |
| CaCl2 | 6.044e-010 | 6.044e-010 | -9.219 | -9.219 | 0.000 | |
| CuCl2 | 3.393e-010 | 3.393e-010 | -9.469 | -9.469 | 0.000 | |
| ZnCl2 | 2.288e-010 | 2.288e-010 | -9.640 | -9.640 | 0.000 | |
| Zn(OH)Cl | 4.517e-012 | 4.517e-012 | -11.345 | -11.345 | 0.000 | |
| FeCl2 | 2.480e-012 | 2.480e-012 | -11.606 | -11.606 | 0.000 | |
| ZnCl3- | 1.655e-013 | 1.385e-013 | -12.781 | -12.858 | -0.077 | |
| MnCl3- | 9.510e-014 | 7.962e-014 | -13.022 | -13.099 | -0.077 | |
| CuCl2- | 1.020e-014 | 8.543e-015 | -13.991 | -14.068 | -0.077 | |
| ZnCl4-2 | 2.368e-015 | 1.151e-015 | -14.626 | -14.939 | -0.313 | |
| CuCl3-2 | 1.237e-016 | 6.015e-017 | -15.908 | -16.221 | -0.313 | |
| FeCl4-2 | 1.771e-017 | 8.612e-018 | -16.752 | -17.065 | -0.313 | |
| FeCl4- | 1.416e-017 | 1.185e-017 | -16.849 | -16.926 | -0.077 | |
| CuCl4-2 | 1.574e-020 | 7.653e-021 | -19.803 | -20.116 | -0.313 | |
| Cl(1) | 4.682e-027 | | | | | |
| HClO | 4.682e-027 | 4.682e-027 | -26.330 | -26.330 | 0.000 | |
| ClO- | 2.230e-031 | 1.867e-031 | -30.652 | -30.729 | -0.077 | |
| Cl(3) | 0.000e+000 | | | | | |
| ClO2- | 0.000e+000 | 0.000e+000 | -51.315 | -51.392 | -0.077 | |
| HClO2 | 0.000e+000 | 0.000e+000 | -51.392 | -51.392 | 0.000 | |
| Cl(5) | 0.000e+000 | | | | | |
| ClO3- | 0.000e+000 | 0.000e+000 | -58.124 | -58.203 | -0.079 | |
| Cl(7) | 0.000e+000 | | | | | |
| ClO4- | 0.000e+000 | 0.000e+000 | -69.237 | -69.316 | -0.079 | |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -71.975 | -72.052 | -0.077 | |
| Cu(1) | 1.385e-013 | | | | | |
| Cu+ | 1.281e-013 | 1.073e-013 | -12.892 | -12.969 | -0.077 | |
| CuCl2- | 1.020e-014 | 8.543e-015 | -13.991 | -14.068 | -0.077 | |
| CuCl3-2 | 1.237e-016 | 6.015e-017 | -15.908 | -16.221 | -0.313 | |
| Cu(2) | 5.533e-004 | | | | | |
| Cu+2 | 3.771e-004 | 1.960e-004 | -3.424 | -3.708 | -0.284 | |
| CuSO4 | 1.755e-004 | 1.755e-004 | -3.756 | -3.756 | 0.000 | |
| CuCl+ | 7.019e-007 | 5.877e-007 | -6.154 | -6.231 | -0.077 | |
| CuOH+ | 1.785e-008 | 1.495e-008 | -7.748 | -7.825 | -0.077 | |
| CuCl2 | 3.393e-010 | 3.393e-010 | -9.469 | -9.469 | 0.000 | |
| CuCl4-2 | 1.574e-020 | 7.653e-021 | -19.803 | -20.116 | -0.313 | |

| | | | | | |
|------------|------------|------------|---------|---------|--------|
| CuO2-2 | 6.844e-031 | 3.328e-031 | -30.165 | -30.478 | -0.313 |
| Fe(2) | 1.343e-003 | | | | |
| Fe+2 | 1.016e-003 | 5.278e-004 | -2.993 | -3.278 | -0.284 |
| FeSO4 | 3.270e-004 | 3.270e-004 | -3.486 | -3.486 | 0.000 |
| FeCl+ | 5.035e-007 | 4.215e-007 | -6.298 | -6.375 | -0.077 |
| FeOH+ | 2.947e-010 | 2.468e-010 | -9.531 | -9.608 | -0.077 |
| FeCl2 | 2.480e-012 | 2.480e-012 | -11.606 | -11.606 | 0.000 |
| FeCl4-2 | 1.771e-017 | 8.612e-018 | -16.752 | -17.065 | -0.313 |
| Fe(OH)2 | 2.898e-018 | 2.898e-018 | -17.538 | -17.538 | 0.000 |
| Fe(OH)3- | 2.037e-025 | 1.706e-025 | -24.691 | -24.768 | -0.077 |
| Fe(OH)4-2 | 5.187e-037 | 2.522e-037 | -36.285 | -36.598 | -0.313 |
| Fe(3) | 1.710e-003 | | | | |
| FeOH+2 | 9.759e-004 | 4.831e-004 | -3.011 | -3.316 | -0.305 |
| Fe(OH)2+ | 2.825e-004 | 2.365e-004 | -3.549 | -3.626 | -0.077 |
| Fe+3 | 1.852e-004 | 5.061e-005 | -3.732 | -4.296 | -0.564 |
| Fe2(OH)2+4 | 9.255e-005 | 6.281e-006 | -4.034 | -5.202 | -1.168 |
| FeSO4+ | 2.286e-005 | 1.914e-005 | -4.641 | -4.718 | -0.077 |
| Fe3(OH)4+5 | 1.889e-005 | 3.104e-007 | -4.724 | -6.508 | -1.784 |
| Fe(SO4)2- | 1.510e-006 | 1.265e-006 | -5.821 | -5.898 | -0.077 |
| Fe(OH)3 | 1.635e-007 | 1.635e-007 | -6.786 | -6.786 | 0.000 |
| FeCl+2 | 1.867e-008 | 9.244e-009 | -7.729 | -8.034 | -0.305 |
| FeCl2+ | 9.799e-009 | 8.204e-009 | -8.009 | -8.086 | -0.077 |
| Fe(OH)4- | 7.254e-014 | 6.074e-014 | -13.139 | -13.217 | -0.077 |
| FeCl4- | 1.416e-017 | 1.185e-017 | -16.849 | -16.926 | -0.077 |
| H(0) | 7.189e-034 | | | | |
| H2 | 3.595e-034 | 3.627e-034 | -33.444 | -33.440 | 0.004 |
| K | 1.773e-003 | | | | |
| K+ | 1.719e-003 | 1.426e-003 | -2.765 | -2.846 | -0.081 |
| KSO4- | 5.372e-005 | 4.497e-005 | -4.270 | -4.347 | -0.077 |
| KCl | 5.248e-008 | 5.248e-008 | -7.280 | -7.280 | 0.000 |
| KHSO4 | 2.683e-008 | 2.683e-008 | -7.571 | -7.571 | 0.000 |
| KOH | 7.308e-015 | 7.308e-015 | -14.136 | -14.136 | 0.000 |
| Mg | 8.161e-004 | | | | |
| Mg+2 | 5.185e-004 | 2.848e-004 | -3.285 | -3.545 | -0.260 |
| MgSO4 | 2.973e-004 | 2.973e-004 | -3.527 | -3.527 | 0.000 |
| MgCl+ | 2.911e-007 | 2.438e-007 | -6.536 | -6.613 | -0.077 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -40.084 | -41.252 | -1.168 |
| Mn(2) | 3.756e-004 | | | | |
| Mn+2 | 2.500e-004 | 1.299e-004 | -3.602 | -3.886 | -0.284 |
| MnSO4 | 1.253e-004 | 1.253e-004 | -3.902 | -3.902 | 0.000 |
| MnCl+ | 3.622e-007 | 3.033e-007 | -6.441 | -6.518 | -0.077 |
| MnOH+ | 5.897e-012 | 4.937e-012 | -11.229 | -11.307 | -0.077 |
| MnCl3- | 9.510e-014 | 7.962e-014 | -13.022 | -13.099 | -0.077 |
| Mn2OH+3 | 3.232e-015 | 6.873e-016 | -14.490 | -15.163 | -0.672 |
| Mn(OH)2 | 1.792e-020 | 1.792e-020 | -19.747 | -19.747 | 0.000 |
| Mn2(OH)3+ | 8.202e-023 | 6.867e-023 | -22.086 | -22.163 | -0.077 |
| Mn(OH)3- | 2.968e-029 | 2.485e-029 | -28.528 | -28.605 | -0.077 |
| Mn(OH)4-2 | 6.398e-040 | 3.111e-040 | -39.194 | -39.507 | -0.313 |
| Mn(3) | 1.630e-017 | | | | |
| Mn+3 | 1.630e-017 | 3.465e-018 | -16.788 | -17.460 | -0.672 |
| Mn(6) | 0.000e+000 | | | | |
| MnO4-2 | 0.000e+000 | 0.000e+000 | -48.661 | -48.974 | -0.313 |
| Mn(7) | 0.000e+000 | | | | |
| MnO4- | 0.000e+000 | 0.000e+000 | -46.251 | -46.330 | -0.079 |
| Na | 1.447e-003 | | | | |
| Na+ | 1.410e-003 | 1.181e-003 | -2.851 | -2.928 | -0.077 |
| NaSO4- | 3.641e-005 | 3.049e-005 | -4.439 | -4.516 | -0.077 |
| NaCl | 2.275e-007 | 2.275e-007 | -6.643 | -6.643 | 0.000 |
| NaOH | 2.901e-015 | 2.901e-015 | -14.537 | -14.537 | 0.000 |
| NaAlO2 | 1.338e-018 | 1.338e-018 | -17.874 | -17.874 | 0.000 |
| O(0) | 9.587e-026 | | | | |
| O2 | 4.793e-026 | 4.837e-026 | -25.319 | -25.315 | 0.004 |
| S(6) | 1.136e-002 | | | | |
| SO4-2 | 8.038e-003 | 3.909e-003 | -2.095 | -2.408 | -0.313 |
| CaSO4 | 1.152e-003 | 1.152e-003 | -2.939 | -2.939 | 0.000 |
| AlSO4+ | 4.577e-004 | 3.832e-004 | -3.339 | -3.417 | -0.077 |
| FeSO4 | 3.270e-004 | 3.270e-004 | -3.486 | -3.486 | 0.000 |

| | | | | | |
|-----------|------------|------------|---------|---------|--------|
| HSO4- | 3.188e-004 | 2.669e-004 | -3.496 | -3.574 | -0.077 |
| MgSO4 | 2.973e-004 | 2.973e-004 | -3.527 | -3.527 | 0.000 |
| CuSO4 | 1.755e-004 | 1.755e-004 | -3.756 | -3.756 | 0.000 |
| Al(SO4)2- | 1.389e-004 | 1.163e-004 | -3.857 | -3.935 | -0.077 |
| MnSO4 | 1.253e-004 | 1.253e-004 | -3.902 | -3.902 | 0.000 |
| ZnSO4 | 7.968e-005 | 7.968e-005 | -4.099 | -4.099 | 0.000 |
| KSO4- | 5.372e-005 | 4.497e-005 | -4.270 | -4.347 | -0.077 |
| NaSO4- | 3.641e-005 | 3.049e-005 | -4.439 | -4.516 | -0.077 |
| FeSO4+ | 2.286e-005 | 1.914e-005 | -4.641 | -4.718 | -0.077 |
| Fe(SO4)2- | 1.510e-006 | 1.265e-006 | -5.821 | -5.898 | -0.077 |
| KHSO4 | 2.683e-008 | 2.683e-008 | -7.571 | -7.571 | 0.000 |
| H2SO4 | 1.703e-010 | 1.703e-010 | -9.769 | -9.769 | 0.000 |
| Zn | 2.666e-004 | | | | |
| Zn+2 | 1.867e-004 | 9.702e-005 | -3.729 | -4.013 | -0.284 |
| ZnSO4 | 7.968e-005 | 7.968e-005 | -4.099 | -4.099 | 0.000 |
| ZnCl+ | 2.134e-007 | 1.787e-007 | -6.671 | -6.748 | -0.077 |
| ZnCl2 | 2.288e-010 | 2.288e-010 | -9.640 | -9.640 | 0.000 |
| ZnOH+ | 1.879e-010 | 1.573e-010 | -9.726 | -9.803 | -0.077 |
| Zn(OH)Cl | 4.517e-012 | 4.517e-012 | -11.345 | -11.345 | 0.000 |
| ZnCl3- | 1.655e-013 | 1.385e-013 | -12.781 | -12.858 | -0.077 |
| ZnCl4-2 | 2.368e-015 | 1.151e-015 | -14.626 | -14.939 | -0.313 |
| Zn(OH)2 | 9.960e-016 | 9.960e-016 | -15.002 | -15.002 | 0.000 |
| Zn(OH)3- | 5.452e-024 | 4.565e-024 | -23.263 | -23.341 | -0.077 |
| Zn(OH)4-2 | 2.366e-033 | 1.151e-033 | -32.626 | -32.939 | -0.313 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -71.975 | -72.052 | -0.077 |

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

| Phase | SI | log IAP | log KT | |
|-------------------|---------|---------|--------|-------------------|
| Al | -125.44 | 24.48 | 149.91 | Al |
| Al(g) | -176.14 | 24.48 | 200.62 | Al |
| Al2(SO4)3 | -34.16 | -15.26 | 18.90 | Al2(SO4)3 |
| Al2(SO4)3:6H2O | -16.82 | -15.26 | 1.56 | Al2(SO4)3:6H2O |
| Alum-K | -6.71 | -11.68 | -4.97 | KAl(SO4)2:12H2O |
| Alunite | -0.23 | -0.70 | -0.47 | KAl3(OH)6(SO4)2 |
| Anhydrite | -0.75 | -5.10 | -4.35 | CaSO4 |
| Antarcticite | -12.71 | -8.62 | 4.09 | CaCl2:6H2O |
| Antlerite | -9.58 | -0.85 | 8.73 | Cu3(SO4)(OH)4 |
| Aphthitalite | -12.39 | -16.28 | -3.89 | NaK3(SO4)2 |
| Arcanite | -6.26 | -8.10 | -1.84 | K2SO4 |
| Arsenolite | -30.83 | -50.68 | -19.84 | As2O3 |
| As | -49.03 | -6.35 | 42.68 | As |
| As2O5 | -17.06 | -14.93 | 2.14 | As2O5 |
| As4O6(cubi) | -61.53 | -101.35 | -39.82 | As4O6 |
| As4O6(mono) | -61.30 | -101.35 | -40.05 | As4O6 |
| Atacamite | -16.00 | -1.73 | 14.26 | Cu4Cl2(OH)6 |
| Bassanite | -1.40 | -5.10 | -3.71 | CaSO4:0.5H2O |
| Birnessite | -68.13 | -153.67 | -85.55 | Mn8O14:5H2O |
| Bischofite | -13.86 | -9.47 | 4.39 | MgCl2:6H2O |
| Bixbyite | -14.94 | -15.90 | -0.96 | Mn2O3 |
| Bloedite | -11.74 | -14.22 | -2.48 | Na2Mg(SO4)2:4H2O |
| Boehmite | -2.06 | 5.49 | 7.55 | AlO2H |
| Brochantite | -13.64 | 1.78 | 15.42 | Cu4(SO4)(OH)6 |
| Brucite | -13.49 | 2.79 | 16.28 | Mg(OH)2 |
| Ca | -123.53 | 16.30 | 139.83 | Ca |
| Ca(g) | -148.77 | 16.30 | 165.07 | Ca |
| Ca2Al2O5:8H2O | -41.30 | 18.27 | 59.57 | Ca2Al2O5:8H2O |
| Ca2Cl2(OH)2:H2O | -31.26 | -4.97 | 26.29 | Ca2Cl2(OH)2:H2O |
| Ca3(AsO4)2 | -21.80 | -3.99 | 17.80 | Ca3(AsO4)2 |
| Ca3Al2O6 | -91.12 | 21.92 | 113.03 | Ca3Al2O6 |
| Ca4Al2Fe2O10 | -104.49 | 35.99 | 140.48 | Ca4Al2Fe2O10 |
| Ca4Al2O7:13H2O | -81.70 | 25.56 | 107.25 | Ca4Al2O7:13H2O |
| Ca4Al2O7:19H2O | -78.12 | 25.56 | 103.68 | Ca4Al2O7:19H2O |
| Ca4Cl2(OH)6:13H2O | -66.01 | 2.32 | 68.33 | Ca4Cl2(OH)6:13H2O |
| CaAl2O4 | -32.28 | 14.63 | 46.91 | CaAl2O4 |
| CaAl2O4:10H2O | -23.37 | 14.63 | 37.99 | CaAl2O4:10H2O |

| | | | | |
|-------------------------|---------|--------|--------|--------------------------|
| CaAl4O7 | -42.98 | 25.61 | 68.59 | CaAl4O7 |
| Carnallite | -19.54 | -15.27 | 4.27 | KMgCl3:6H2O |
| CaSO4:0.5H2O(beta) | -1.57 | -5.10 | -3.54 | CaSO4:0.5H2O |
| Chalcanthite | -3.49 | -6.12 | -2.63 | CuSO4:5H2O |
| Chalcocyanite | -9.03 | -6.12 | 2.91 | CuSO4 |
| Chloromagnesite | -31.28 | -9.47 | 21.82 | MgCl2 |
| Cl2(g) | -27.91 | -24.92 | 2.99 | Cl2 |
| Claudetite | -30.88 | -50.68 | -19.80 | As2O3 |
| Corundum | -7.31 | 10.98 | 18.29 | Al2O3 |
| Cu | -16.21 | 15.29 | 31.50 | Cu |
| Cu(g) | -68.37 | 15.29 | 83.66 | Cu |
| CuCl2 | -13.35 | -9.63 | 3.72 | CuCl2 |
| Cuprite | -17.69 | -19.60 | -1.91 | Cu2O |
| Delafossite | 1.85 | -4.59 | -6.44 | CuFeO2 |
| Diaspore | -1.66 | 5.49 | 7.15 | AlHO2 |
| Epsomite | -3.99 | -5.95 | -1.96 | MgSO4:7H2O |
| Ettringite | -55.86 | 6.60 | 62.46 | Ca6Al2(SO4)3(OH)12:26H2O |
| Fe | -43.30 | 15.72 | 59.02 | Fe |
| Fe(OH)2 | -10.83 | 3.06 | 13.89 | Fe(OH)2 |
| Fe(OH)3 | -0.43 | 5.21 | 5.64 | Fe(OH)3 |
| Fe2(SO4)3 | -18.86 | -15.82 | 3.05 | Fe2(SO4)3 |
| FeO | -10.46 | 3.06 | 13.52 | FeO |
| Ferrite-Ca | -7.42 | 14.07 | 21.50 | CaFe2O4 |
| Ferrite-Cu | 2.78 | 13.06 | 10.28 | CuFe2O4 |
| Ferrite-Dicalcium | -39.08 | 17.72 | 56.80 | Ca2Fe2O5 |
| Ferrite-Mg | -7.80 | 13.22 | 21.02 | MgFe2O4 |
| Ferrite-Zn | 1.05 | 12.75 | 11.70 | ZnFe2O4 |
| FeSO4 | -8.29 | -5.69 | 2.61 | FeSO4 |
| Gibbsite | -2.25 | 5.49 | 7.74 | Al(OH)3 |
| Glauberite | -7.90 | -13.37 | -5.47 | Na2Ca(SO4)2 |
| Goethite | 4.68 | 5.21 | 0.53 | FeOOH |
| Gypsum | -0.57 | -5.10 | -4.53 | CaSO4:2H2O |
| H2(g) | -30.34 | -33.44 | -3.10 | H2 |
| H2O(g) | -1.59 | -0.00 | 1.59 | H2O |
| Halite | -7.45 | -5.89 | 1.56 | NaCl |
| Hausmannite | -23.59 | -13.45 | 10.14 | Mn3O4 |
| HCl(g) | -12.43 | -6.13 | 6.30 | HCl |
| Hematite | 10.35 | 10.43 | 0.08 | Fe2O3 |
| Hercynite | -14.76 | 14.04 | 28.80 | FeAl2O4 |
| Hexahydrite | -4.23 | -5.95 | -1.73 | MgSO4:6H2O |
| Hydrophilite | -20.36 | -8.62 | 11.75 | CaCl2 |
| Ice | -0.14 | -0.00 | 0.14 | H2O |
| Jarosite | 7.88 | -1.53 | -9.41 | KFe3(SO4)2(OH)6 |
| Jarosite-Na | 3.84 | -1.61 | -5.45 | NaFe3(SO4)2(OH)6 |
| K | -64.32 | 6.65 | 70.98 | K |
| K(g) | -74.93 | 6.65 | 81.58 | K |
| K2O | -83.39 | 0.65 | 84.04 | K2O |
| K3H(SO4)2 | -12.90 | -16.52 | -3.62 | K3H(SO4)2 |
| Kainite | -11.45 | -11.76 | -0.31 | KMgClSO4:3H2O |
| KAl(SO4)2 | -14.95 | -11.68 | 3.27 | KAl(SO4)2 |
| Katoite | -57.03 | 21.91 | 78.94 | Ca3Al2H12O12 |
| Kieserite | -5.69 | -5.95 | -0.27 | MgSO4:H2O |
| KMgCl3 | -36.52 | -15.27 | 21.25 | KMgCl3 |
| KMgCl3:2H2O | -29.23 | -15.27 | 13.96 | KMgCl3:2H2O |
| Lammerite | -8.58 | -7.03 | 1.55 | Cu3(AsO4)2 |
| Lawrencite | -18.25 | -9.20 | 9.05 | FeCl2 |
| Leonite | -9.94 | -14.05 | -4.11 | K2Mg(SO4)2:4H2O |
| Lime | -28.92 | 3.64 | 32.57 | CaO |
| Magnetite | 3.07 | 13.49 | 10.42 | Fe3O4 |
| Manganite | -7.79 | -7.95 | -0.16 | MnO(OH) |
| Manganosite | -15.46 | 2.45 | 17.92 | MnO |
| Mayenite | -373.54 | 120.61 | 494.15 | Ca12Al14O33 |
| Melanterite | -3.29 | -5.69 | -2.40 | FeSO4:7H2O |
| Mercallite | -6.99 | -8.42 | -1.44 | KHSO4 |
| Mg | -107.07 | 15.45 | 122.52 | Mg |
| Mg(g) | -126.79 | 15.45 | 142.25 | Mg |
| Mg1.25SO4(OH)0.5:0.5H2O | -10.45 | -5.25 | 5.20 | Mg1.25SO4(OH)0.5:0.5H2O |

| | | | | |
|------------------|---------|---------|--------|--------------------|
| Mg1.5SO4(OH) | -13.77 | -4.56 | 9.21 | Mg1.5SO4(OH) |
| MgCl2:2H2O | -22.20 | -9.47 | 12.73 | MgCl2:2H2O |
| MgCl2:4H2O | -16.77 | -9.47 | 7.30 | MgCl2:4H2O |
| MgCl2:H2O | -25.54 | -9.47 | 16.07 | MgCl2:H2O |
| MgOHCl | -19.23 | -3.34 | 15.89 | MgOHCl |
| MgSO4 | -10.78 | -5.95 | 4.83 | MgSO4 |
| Mirabilite | -7.11 | -8.27 | -1.15 | Na2SO4:10H2O |
| Misenite | -47.57 | -58.64 | -11.08 | K8H6(SO4)7 |
| Mn | -67.82 | 15.11 | 82.93 | Mn |
| Mn(OH)2(am) | -12.85 | 2.45 | 15.31 | Mn(OH)2 |
| Mn(OH)3 | -14.29 | -7.95 | 6.34 | Mn(OH)3 |
| MnCl2:2H2O | -13.80 | -9.81 | 4.00 | MnCl2:2H2O |
| MnCl2:4H2O | -12.56 | -9.81 | 2.75 | MnCl2:4H2O |
| MnCl2:H2O | -15.35 | -9.81 | 5.54 | MnCl2:H2O |
| MnO2(gamma) | -10.30 | -26.43 | -16.13 | MnO2 |
| MnSO4 | -8.90 | -6.29 | 2.61 | MnSO4 |
| Molysite | -26.65 | -13.18 | 13.47 | FeCl3 |
| Na | -60.80 | 6.57 | 67.37 | Na |
| Na(g) | -74.29 | 6.57 | 80.86 | Na |
| Na2O | -66.93 | 0.48 | 67.42 | Na2O |
| Na3H(SO4)2 | -15.88 | -16.77 | -0.89 | Na3H(SO4)2 |
| Na4Ca(SO4)3:2H2O | -15.74 | -21.63 | -5.89 | Na4Ca(SO4)3:2H2O |
| NaFeO2 | -14.43 | 5.46 | 19.88 | NaFeO2 |
| Nantokite | -9.16 | -15.93 | -6.77 | CuCl |
| O2(g) | -22.42 | -25.32 | -2.89 | O2 |
| Oxychloride-Mg | -26.37 | -0.54 | 25.83 | Mg2Cl(OH)3:4H2O |
| Pentahydrate | -4.57 | -5.95 | -1.39 | MgSO4:5H2O |
| Periclase | -18.53 | 2.79 | 21.33 | MgO |
| Picromerite | -9.61 | -14.05 | -4.44 | K2Mg(SO4)2:6H2O |
| Polyhalite | -9.95 | -24.26 | -14.31 | K2MgCa2(SO4)4:2H2O |
| Portlandite | -18.90 | 3.64 | 22.55 | Ca(OH)2 |
| Pyrolusite | -8.77 | -26.43 | -17.66 | MnO2 |
| Scacchite | -18.55 | -9.81 | 8.74 | MnCl2 |
| Spinel | -23.83 | 13.78 | 37.61 | Al2MgO4 |
| Starkeyite | -4.95 | -5.95 | -1.00 | MgSO4:4H2O |
| Sylvite | -6.63 | -5.81 | 0.83 | KCl |
| Syngenite | -5.60 | -13.20 | -7.60 | K2Ca(SO4)2:H2O |
| Tachyhydrite | -44.69 | -27.55 | 17.14 | Mg2CaCl6:12H2O |
| Tenorite | -5.01 | 2.63 | 7.65 | CuO |
| Thenardite | -7.91 | -8.26 | -0.36 | Na2SO4 |
| Todorokite | -57.19 | -103.02 | -45.82 | Mn7O12:3H2O |
| Wustite | -9.27 | 3.13 | 12.40 | Fe.9470 |
| Zincite | -8.87 | 2.33 | 11.20 | ZnO |
| Zn | -53.80 | 14.98 | 68.79 | Zn |
| Zn(ClO4)2:6H2O | -148.28 | -142.65 | 5.63 | Zn(ClO4)2:6H2O |
| Zn(g) | -70.42 | 14.98 | 85.41 | Zn |
| Zn(OH)2(beta) | -9.61 | 2.33 | 11.93 | Zn(OH)2 |
| Zn(OH)2(epsilon) | -9.33 | 2.33 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -9.56 | 2.33 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -16.77 | -1.48 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -11.68 | -4.09 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -17.26 | -7.95 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -29.61 | -10.52 | 19.09 | Zn3O(SO4)2 |
| ZnCl2 | -17.01 | -9.93 | 7.08 | ZnCl2 |
| ZnSO4 | -9.95 | -6.42 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -4.72 | -6.42 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -4.54 | -6.42 | -1.88 | ZnSO4:7H2O |
| ZnSO4:H2O | -5.87 | -6.42 | -0.55 | ZnSO4:H2O |

Initial solution 3. AS2

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

| Elements | Molality | Moles |
|----------|------------|------------|
| As | 2.041e-006 | 2.041e-006 |
| C(4) | 2.525e-003 | 2.525e-003 |

| | | |
|------|------------|------------|
| Ca | 5.958e-003 | 5.958e-003 |
| Cl | 1.918e-002 | 1.918e-002 |
| K | 1.044e-003 | 1.044e-003 |
| Mg | 5.644e-004 | 5.644e-004 |
| Mn | 2.079e-006 | 2.079e-006 |
| Na | 1.712e-002 | 1.712e-002 |
| S(6) | 4.455e-003 | 4.455e-003 |
| Zn | 3.739e-005 | 3.739e-005 |

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

| | | |
|--|---|---------------|
| pH | = | 6.980 |
| pe | = | 10.000 |
| Activity of water | = | 0.999 |
| Ionic strength | = | 3.800e-002 |
| Mass of water (kg) | = | 1.000e+000 |
| Total alkalinity (eq/kg) | = | 2.128e-003 |
| Total CO2 (mol/kg) | = | 2.525e-003 |
| Temperature (deg C) | = | 25.000 |
| Electrical balance (eq) | = | 1.075e-003 |
| Percent error, 100*(Cat- An)/(Cat+ An) | = | 1.86 |
| Iterations | = | 4 |
| Total H | = | 1.110528e+002 |
| Total O | = | 5.555032e+001 |

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|----------|------------|------------|--------------|--------------|-----------|
| H+ | 1.207e-007 | 1.047e-007 | -6.918 | -6.980 | -0.062 |
| OH- | 1.105e-007 | 9.193e-008 | -6.957 | -7.037 | -0.080 |
| H2O | 5.553e+001 | 9.992e-001 | 1.744 | -0.000 | 0.000 |
| As(-3) | 0.000e+000 | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -132.370 | -132.370 | 0.000 |
| As(3) | 5.398e-026 | | | | |
| HAsO2 | 2.863e-026 | 2.863e-026 | -25.543 | -25.543 | 0.000 |
| As(OH)3 | 2.501e-026 | 2.501e-026 | -25.602 | -25.602 | 0.000 |
| H2AsO3- | 1.747e-028 | 1.461e-028 | -27.758 | -27.835 | -0.078 |
| AsO2- | 1.672e-028 | 1.398e-028 | -27.777 | -27.855 | -0.078 |
| AsO2OH-2 | 2.820e-032 | 1.363e-032 | -31.550 | -31.866 | -0.316 |
| As(5) | 2.041e-006 | | | | |
| HAsO4-2 | 1.495e-006 | 7.226e-007 | -5.825 | -6.141 | -0.316 |
| H2AsO4- | 5.453e-007 | 4.559e-007 | -6.263 | -6.341 | -0.078 |
| AsO4-3 | 9.134e-011 | 1.770e-011 | -10.039 | -10.752 | -0.713 |
| H3AsO4 | 8.408e-012 | 8.408e-012 | -11.075 | -11.075 | 0.000 |
| C(4) | 2.525e-003 | | | | |
| HCO3- | 2.009e-003 | 1.680e-003 | -2.697 | -2.775 | -0.078 |
| CO2 | 4.046e-004 | 4.084e-004 | -3.393 | -3.389 | 0.004 |
| CaHCO3+ | 6.422e-005 | 5.369e-005 | -4.192 | -4.270 | -0.078 |
| NaHCO3 | 3.387e-005 | 3.387e-005 | -4.470 | -4.470 | 0.000 |
| MgHCO3+ | 5.687e-006 | 4.755e-006 | -5.245 | -5.323 | -0.078 |
| CaCO3 | 4.449e-006 | 4.449e-006 | -5.352 | -5.352 | 0.000 |
| CO3-2 | 1.446e-006 | 7.117e-007 | -5.840 | -6.148 | -0.308 |
| ZnHCO3+ | 8.088e-007 | 6.762e-007 | -6.092 | -6.170 | -0.078 |
| MgCO3 | 1.835e-007 | 1.835e-007 | -6.736 | -6.736 | 0.000 |
| ZnCO3 | 9.333e-008 | 9.333e-008 | -7.030 | -7.030 | 0.000 |
| NaCO3- | 4.199e-008 | 3.511e-008 | -7.377 | -7.455 | -0.078 |
| MnCO3 | 2.132e-008 | 2.132e-008 | -7.671 | -7.671 | 0.000 |
| MnHCO3+ | 1.309e-008 | 1.095e-008 | -7.883 | -7.961 | -0.078 |
| Ca | 5.958e-003 | | | | |
| Ca+2 | 5.216e-003 | 2.697e-003 | -2.283 | -2.569 | -0.286 |
| CaSO4 | 6.619e-004 | 6.619e-004 | -3.179 | -3.179 | 0.000 |
| CaHCO3+ | 6.422e-005 | 5.369e-005 | -4.192 | -4.270 | -0.078 |
| CaCl+ | 1.082e-005 | 9.048e-006 | -4.966 | -5.043 | -0.078 |
| CaCO3 | 4.449e-006 | 4.449e-006 | -5.352 | -5.352 | 0.000 |
| CaCl2 | 1.685e-007 | 1.685e-007 | -6.774 | -6.774 | 0.000 |

| | | | | | |
|------------|------------|------------|---------|---------|--------|
| CaOH+ | 4.348e-009 | 3.635e-009 | -8.362 | -8.439 | -0.078 |
| Cl(-1) | 1.918e-002 | | | | |
| Cl- | 1.912e-002 | 1.583e-002 | -1.719 | -1.801 | -0.082 |
| NaCl | 3.922e-005 | 3.922e-005 | -4.407 | -4.407 | 0.000 |
| CaCl+ | 1.082e-005 | 9.048e-006 | -4.966 | -5.043 | -0.078 |
| MgCl+ | 3.602e-006 | 3.011e-006 | -5.443 | -5.521 | -0.078 |
| ZnCl+ | 4.967e-007 | 4.153e-007 | -6.304 | -6.382 | -0.078 |
| KCl | 4.530e-007 | 4.530e-007 | -6.344 | -6.344 | 0.000 |
| CaCl2 | 1.685e-007 | 1.685e-007 | -6.774 | -6.774 | 0.000 |
| Zn(OH)Cl | 6.775e-008 | 6.775e-008 | -7.169 | -7.169 | 0.000 |
| MnCl+ | 3.450e-008 | 2.885e-008 | -7.462 | -7.540 | -0.078 |
| ZnCl2 | 7.678e-009 | 7.678e-009 | -8.115 | -8.115 | 0.000 |
| HCl | 3.723e-010 | 3.723e-010 | -9.429 | -9.429 | 0.000 |
| ZnCl3- | 8.028e-011 | 6.712e-011 | -10.095 | -10.173 | -0.078 |
| ZnCl4-2 | 1.666e-011 | 8.053e-012 | -10.778 | -11.094 | -0.316 |
| MnCl3- | 1.888e-012 | 1.579e-012 | -11.724 | -11.802 | -0.078 |
| Cl(1) | 5.707e-026 | | | | |
| HClO | 4.363e-026 | 4.363e-026 | -25.360 | -25.360 | 0.000 |
| ClO- | 1.344e-026 | 1.124e-026 | -25.872 | -25.949 | -0.078 |
| Cl(3) | 0.000e+000 | | | | |
| ClO2- | 0.000e+000 | 0.000e+000 | -42.915 | -42.993 | -0.078 |
| HClO2 | 0.000e+000 | 0.000e+000 | -46.803 | -46.803 | 0.000 |
| Cl(5) | 0.000e+000 | | | | |
| ClO3- | 0.000e+000 | 0.000e+000 | -46.104 | -46.184 | -0.080 |
| Cl(7) | 0.000e+000 | | | | |
| ClO4- | 0.000e+000 | 0.000e+000 | -53.597 | -53.677 | -0.080 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -57.129 | -57.207 | -0.078 |
| H(0) | 1.724e-037 | | | | |
| H2 | 8.621e-038 | 8.701e-038 | -37.064 | -37.060 | 0.004 |
| K | 1.044e-003 | | | | |
| K+ | 1.029e-003 | 8.522e-004 | -2.987 | -3.069 | -0.082 |
| KSO4- | 1.382e-005 | 1.156e-005 | -4.859 | -4.937 | -0.078 |
| KCl | 4.530e-007 | 4.530e-007 | -6.344 | -6.344 | 0.000 |
| KOH | 2.820e-011 | 2.820e-011 | -10.550 | -10.550 | 0.000 |
| KHSO4 | 1.068e-012 | 1.068e-012 | -11.972 | -11.972 | 0.000 |
| Mg | 5.644e-004 | | | | |
| Mg+2 | 4.456e-004 | 2.437e-004 | -3.351 | -3.613 | -0.262 |
| MgSO4 | 1.093e-004 | 1.093e-004 | -3.961 | -3.961 | 0.000 |
| MgHCO3+ | 5.687e-006 | 4.755e-006 | -5.245 | -5.323 | -0.078 |
| MgCl+ | 3.602e-006 | 3.011e-006 | -5.443 | -5.521 | -0.078 |
| MgCO3 | 1.835e-007 | 1.835e-007 | -6.736 | -6.736 | 0.000 |
| Mg4(OH)4+4 | 7.829e-026 | 5.199e-027 | -25.106 | -26.284 | -1.178 |
| Mn(2) | 2.079e-006 | | | | |
| Mn+2 | 1.655e-006 | 8.558e-007 | -5.781 | -6.068 | -0.286 |
| MnSO4 | 3.548e-007 | 3.548e-007 | -6.450 | -6.450 | 0.000 |
| MnCl+ | 3.450e-008 | 2.885e-008 | -7.462 | -7.540 | -0.078 |
| MnCO3 | 2.132e-008 | 2.132e-008 | -7.671 | -7.671 | 0.000 |
| MnHCO3+ | 1.309e-008 | 1.095e-008 | -7.883 | -7.961 | -0.078 |
| MnOH+ | 2.511e-010 | 2.099e-010 | -9.600 | -9.678 | -0.078 |
| MnCl3- | 1.888e-012 | 1.579e-012 | -11.724 | -11.802 | -0.078 |
| Mn(OH)2 | 4.917e-015 | 4.917e-015 | -14.308 | -14.308 | 0.000 |
| Mn2(OH)3+ | 9.583e-016 | 8.011e-016 | -15.019 | -15.096 | -0.078 |
| Mn2OH+3 | 9.169e-016 | 1.925e-016 | -15.038 | -15.716 | -0.678 |
| Mn(OH)3- | 5.264e-020 | 4.400e-020 | -19.279 | -19.357 | -0.078 |
| Mn(OH)4-2 | 7.358e-027 | 3.556e-027 | -26.133 | -26.449 | -0.316 |
| Mn(3) | 1.087e-021 | | | | |
| Mn+3 | 1.087e-021 | 2.283e-022 | -20.964 | -21.642 | -0.678 |
| Mn(6) | 4.364e-029 | | | | |
| MnO4-2 | 4.364e-029 | 2.109e-029 | -28.360 | -28.676 | -0.316 |
| Mn(7) | 1.116e-028 | | | | |
| MnO4- | 1.116e-028 | 9.286e-029 | -27.952 | -28.032 | -0.080 |
| Na | 1.712e-002 | | | | |
| Na+ | 1.686e-002 | 1.410e-002 | -1.773 | -1.851 | -0.078 |
| NaSO4- | 1.872e-004 | 1.565e-004 | -3.728 | -3.806 | -0.078 |
| NaCl | 3.922e-005 | 3.922e-005 | -4.407 | -4.407 | 0.000 |
| NaHCO3 | 3.387e-005 | 3.387e-005 | -4.470 | -4.470 | 0.000 |
| NaCO3- | 4.199e-008 | 3.511e-008 | -7.377 | -7.455 | -0.078 |

| | | | | | |
|-----------|------------|------------|---------|---------|--------|
| NaOH | 2.236e-010 | 2.236e-010 | -9.651 | -9.651 | 0.000 |
| O(0) | 1.664e-018 | | | | |
| O2 | 8.321e-019 | 8.398e-019 | -18.080 | -18.076 | 0.004 |
| S(6) | 4.455e-003 | | | | |
| SO4-2 | 3.477e-003 | 1.680e-003 | -2.459 | -2.775 | -0.316 |
| CaSO4 | 6.619e-004 | 6.619e-004 | -3.179 | -3.179 | 0.000 |
| NaSO4- | 1.872e-004 | 1.565e-004 | -3.728 | -3.806 | -0.078 |
| MgSO4 | 1.093e-004 | 1.093e-004 | -3.961 | -3.961 | 0.000 |
| KSO4- | 1.382e-005 | 1.156e-005 | -4.859 | -4.937 | -0.078 |
| ZnSO4 | 5.512e-006 | 5.512e-006 | -5.259 | -5.259 | 0.000 |
| MnSO4 | 3.548e-007 | 3.548e-007 | -6.450 | -6.450 | 0.000 |
| HSO4- | 2.126e-008 | 1.777e-008 | -7.673 | -7.750 | -0.078 |
| KHSO4 | 1.068e-012 | 1.068e-012 | -11.972 | -11.972 | 0.000 |
| H2SO4 | 1.756e-018 | 1.756e-018 | -17.756 | -17.756 | 0.000 |
| Zn | 3.739e-005 | | | | |
| Zn+2 | 3.020e-005 | 1.561e-005 | -4.520 | -4.806 | -0.286 |
| ZnSO4 | 5.512e-006 | 5.512e-006 | -5.259 | -5.259 | 0.000 |
| ZnHCO3+ | 8.088e-007 | 6.762e-007 | -6.092 | -6.170 | -0.078 |
| ZnCl+ | 4.967e-007 | 4.153e-007 | -6.304 | -6.382 | -0.078 |
| ZnOH+ | 1.955e-007 | 1.634e-007 | -6.709 | -6.787 | -0.078 |
| ZnCO3 | 9.333e-008 | 9.333e-008 | -7.030 | -7.030 | 0.000 |
| Zn(OH)Cl | 6.775e-008 | 6.775e-008 | -7.169 | -7.169 | 0.000 |
| ZnCl2 | 7.678e-009 | 7.678e-009 | -8.115 | -8.115 | 0.000 |
| Zn(OH)2 | 6.677e-009 | 6.677e-009 | -8.175 | -8.175 | 0.000 |
| ZnCl3- | 8.028e-011 | 6.712e-011 | -10.095 | -10.173 | -0.078 |
| ZnCl4-2 | 1.666e-011 | 8.053e-012 | -10.778 | -11.094 | -0.316 |
| Zn(OH)3- | 2.362e-013 | 1.975e-013 | -12.627 | -12.704 | -0.078 |
| Zn(OH)4-2 | 6.648e-019 | 3.213e-019 | -18.177 | -18.493 | -0.316 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -57.129 | -57.207 | -0.078 |

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

| Phase | SI | log IAP | log KT | |
|--------------------|---------|---------|--------|-------------------|
| Anhydrite | -0.99 | -5.34 | -4.35 | CaSO4 |
| Antarcticite | -10.27 | -6.17 | 4.09 | CaCl2:6H2O |
| Aphthitalite | -12.72 | -16.61 | -3.89 | NaK3(SO4)2 |
| Aragonite | -0.33 | 1.64 | 1.97 | CaCO3 |
| Arcanite | -7.07 | -8.91 | -1.84 | K2SO4 |
| Arsenolite | -49.79 | -69.63 | -19.84 | As2O3 |
| Artinite | -8.69 | 10.94 | 19.63 | Mg2CO3(OH)2:3H2O |
| As | -63.94 | -21.26 | 42.68 | As |
| As2O5 | -28.78 | -26.64 | 2.14 | As2O5 |
| As4O6(cubi) | -99.44 | -139.26 | -39.82 | As4O6 |
| As4O6(mono) | -99.21 | -139.26 | -40.05 | As4O6 |
| Bassanite | -1.64 | -5.34 | -3.71 | CaSO4:0.5H2O |
| Birnessite | -2.90 | -88.45 | -85.55 | Mn8O14:5H2O |
| Bischofite | -11.61 | -7.22 | 4.39 | MgCl2:6H2O |
| Bixbyite | -0.44 | -1.40 | -0.96 | Mn2O3 |
| Bloedite | -10.39 | -12.87 | -2.48 | Na2Mg(SO4)2:4H2O |
| Brucite | -5.94 | 10.35 | 16.28 | Mg(OH)2 |
| Burkeite | -21.94 | -12.45 | 9.49 | Na6CO3(SO4)2 |
| C | -55.82 | 8.32 | 64.15 | C |
| C(g) | -173.44 | 8.32 | 181.77 | C |
| Ca | -119.40 | 20.43 | 139.83 | Ca |
| Ca(g) | -144.64 | 20.43 | 165.07 | Ca |
| Ca2Cl2(OH)2:H2O | -21.07 | 5.22 | 26.29 | Ca2Cl2(OH)2:H2O |
| Ca3(AsO4)2 | -10.27 | 7.53 | 17.80 | Ca3(AsO4)2 |
| Ca4Cl2(OH)6:13H2O | -40.33 | 28.00 | 68.33 | Ca4Cl2(OH)6:13H2O |
| Calcite | -0.19 | 1.64 | 1.82 | CaCO3 |
| Carnallite | -16.36 | -12.09 | 4.27 | KMgCl3:6H2O |
| CaSO4:0.5H2O(beta) | -1.81 | -5.34 | -3.54 | CaSO4:0.5H2O |
| Chloromagnesite | -29.03 | -7.21 | 21.82 | MgCl2 |
| Cl2(g) | -29.59 | -26.60 | 2.99 | Cl2 |
| Claudetite | -49.83 | -69.63 | -19.80 | As2O3 |
| CO2(g) | -1.93 | -9.75 | -7.83 | CO2 |
| Dolomite | -0.25 | 2.23 | 2.47 | CaMg(CO3)2 |

| | | | | |
|--|---------|--------|--------|--|
| Dolomite-dis | -1.78 | 2.23 | 4.01 | CaMg(CO ₃) ₂ |
| Dolomite-ord | -0.24 | 2.23 | 2.46 | CaMg(CO ₃) ₂ |
| Epsomite | -4.43 | -6.39 | -1.96 | MgSO ₄ :7H ₂ O |
| Gaylussite | -9.03 | 2.14 | 11.16 | CaNa ₂ (CO ₃) ₂ :5H ₂ O |
| Glauberite | -6.35 | -11.82 | -5.47 | Na ₂ Ca(SO ₄) ₂ |
| Gypsum | -0.81 | -5.34 | -4.53 | CaSO ₄ :2H ₂ O |
| H ₂ (g) | -33.96 | -37.06 | -3.10 | H ₂ |
| H ₂ O(g) | -1.59 | -0.00 | 1.59 | H ₂ O |
| Halite | -5.21 | -3.65 | 1.56 | NaCl |
| Hausmannite | -3.66 | 6.49 | 10.14 | Mn ₃ O ₄ |
| HCl(g) | -15.08 | -8.78 | 6.30 | HCl |
| Hexahydrate | -4.66 | -6.39 | -1.73 | MgSO ₄ :6H ₂ O |
| Huntite | -6.81 | 3.41 | 10.22 | CaMg ₃ (CO ₃) ₄ |
| Hydromagnesite | -18.03 | 12.71 | 30.74 | Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O |
| Hydrophilite | -17.92 | -6.17 | 11.75 | CaCl ₂ |
| Hydrozincite | -4.05 | 26.26 | 30.31 | Zn ₅ (OH) ₆ (CO ₃) ₂ |
| Ice | -0.14 | -0.00 | 0.14 | H ₂ O |
| K | -62.55 | 8.43 | 70.98 | K |
| K(g) | -73.15 | 8.43 | 81.58 | K |
| K ₂ CO ₃ :1.5H ₂ O | -15.31 | -1.93 | 13.38 | K ₂ CO ₃ :1.5H ₂ O |
| K ₂ O | -76.21 | 7.82 | 84.04 | K ₂ O |
| K ₃ H(SO ₄) ₂ | -18.11 | -21.74 | -3.62 | K ₃ H(SO ₄) ₂ |
| K ₈ H ₄ (CO ₃) ₆ :3H ₂ O | -54.95 | -27.24 | 27.71 | K ₈ H ₄ (CO ₃) ₆ :3H ₂ O |
| Kainite | -10.95 | -11.26 | -0.31 | KMgClSO ₄ :3H ₂ O |
| Kaliginite | -6.13 | -5.84 | 0.28 | KHCO ₃ |
| Kieserite | -6.12 | -6.39 | -0.27 | MgSO ₄ :H ₂ O |
| KMgCl ₃ | -33.33 | -12.08 | 21.25 | KMgCl ₃ |
| KMgCl ₃ :2H ₂ O | -26.05 | -12.08 | 13.96 | KMgCl ₃ :2H ₂ O |
| KNaCO ₃ :6H ₂ O | -10.98 | -0.72 | 10.26 | KNaCO ₃ :6H ₂ O |
| Lansfordite | -4.25 | 0.59 | 4.84 | MgCO ₃ :5H ₂ O |
| Leonite | -11.19 | -15.30 | -4.11 | K ₂ Mg(SO ₄) ₂ :4H ₂ O |
| Lime | -21.18 | 11.39 | 32.57 | CaO |
| Magnesite | -1.68 | 0.59 | 2.27 | MgCO ₃ |
| Manganite | -0.54 | -0.70 | -0.16 | MnO(OH) |
| Manganosite | -10.02 | 7.89 | 17.92 | MnO |
| Mercallite | -11.39 | -12.82 | -1.44 | KHSO ₄ |
| Mg | -103.14 | 19.38 | 122.52 | Mg |
| Mg(g) | -122.86 | 19.38 | 142.25 | Mg |
| Mg _{1.25} SO ₄ (OH) _{0.5} :0.5H ₂ O | -9.00 | -3.80 | 5.20 | Mg _{1.25} SO ₄ (OH) _{0.5} :0.5H ₂ O |
| Mg _{1.5} SO ₄ (OH) | -10.42 | -1.21 | 9.21 | Mg _{1.5} SO ₄ (OH) |
| MgCl ₂ :2H ₂ O | -19.95 | -7.21 | 12.73 | MgCl ₂ :2H ₂ O |
| MgCl ₂ :4H ₂ O | -14.52 | -7.22 | 7.30 | MgCl ₂ :4H ₂ O |
| MgCl ₂ :H ₂ O | -23.29 | -7.21 | 16.07 | MgCl ₂ :H ₂ O |
| MgOHCl | -14.33 | 1.57 | 15.89 | MgOHCl |
| MgSO ₄ | -11.22 | -6.39 | 4.83 | MgSO ₄ |
| Mirabilite | -5.33 | -6.48 | -1.15 | Na ₂ SO ₄ :10H ₂ O |
| Misenite | -74.78 | -85.86 | -11.08 | K ₈ H ₆ (SO ₄) ₇ |
| Mn | -66.00 | 16.93 | 82.93 | Mn |
| Mn(OH) ₂ (am) | -7.42 | 7.89 | 15.31 | Mn(OH) ₂ |
| Mn(OH) ₃ | -7.04 | -0.70 | 6.34 | Mn(OH) ₃ |
| MnCl ₂ :2H ₂ O | -13.67 | -9.67 | 4.00 | MnCl ₂ :2H ₂ O |
| MnCl ₂ :4H ₂ O | -12.42 | -9.67 | 2.75 | MnCl ₂ :4H ₂ O |
| MnCl ₂ :H ₂ O | -15.21 | -9.67 | 5.54 | MnCl ₂ :H ₂ O |
| MnO ₂ (gamma) | -1.25 | -17.37 | -16.13 | MnO ₂ |
| MnSO ₄ | -11.45 | -8.84 | 2.61 | MnSO ₄ |
| Monohydrocalcite | -1.04 | 1.64 | 2.68 | CaCO ₃ :H ₂ O |
| Na | -57.72 | 9.65 | 67.37 | Na |
| Na(g) | -71.21 | 9.65 | 80.86 | Na |
| Na ₂ CO ₃ | -10.66 | 0.50 | 11.16 | Na ₂ CO ₃ |
| Na ₂ CO ₃ :7H ₂ O | -9.44 | 0.50 | 9.94 | Na ₂ CO ₃ :7H ₂ O |
| Na ₂ O | -57.16 | 10.26 | 67.42 | Na ₂ O |
| Na ₃ H(SO ₄) ₂ | -17.19 | -18.08 | -0.89 | Na ₃ H(SO ₄) ₂ |
| Na ₄ Ca(SO ₄) ₃ :2H ₂ O | -12.40 | -18.30 | -5.89 | Na ₄ Ca(SO ₄) ₃ :2H ₂ O |
| Nahcolite | -4.48 | -4.63 | -0.14 | NaHCO ₃ |
| Natron | -9.09 | 0.50 | 9.59 | Na ₂ CO ₃ :10H ₂ O |
| Nesquehonite | -4.70 | 0.59 | 5.29 | MgCO ₃ :3H ₂ O |
| O ₂ (g) | -15.18 | -18.08 | -2.89 | O ₂ |

| | | | | |
|------------------|---------|---------|--------|--------------------|
| Oxychloride-Mg | -13.92 | 11.91 | 25.83 | Mg2Cl(OH)3:4H2O |
| Pentahydrate | -5.00 | -6.39 | -1.39 | MgSO4:5H2O |
| Periclase | -10.98 | 10.35 | 21.33 | MgO |
| Picromerite | -10.86 | -15.30 | -4.44 | K2Mg(SO4)2:6H2O |
| Pirssonite | -9.18 | 2.14 | 11.32 | Na2Ca(CO3)2:2H2O |
| Polyhalite | -11.68 | -25.99 | -14.31 | K2MgCa2(SO4)4:2H2O |
| Portlandite | -11.16 | 11.39 | 22.55 | Ca(OH)2 |
| Pyrolusite | 0.29 | -17.37 | -17.66 | MnO2 |
| Rhodochrosite | -1.64 | -1.86 | -0.22 | MnCO3 |
| Scacchite | -18.41 | -9.67 | 8.74 | MnCl2 |
| Smithsonite | -1.05 | -0.60 | 0.44 | ZnCO3 |
| Starkeyite | -5.39 | -6.39 | -1.00 | MgSO4:4H2O |
| Sylvite | -5.70 | -4.87 | 0.83 | KCl |
| Syngenite | -6.66 | -14.26 | -7.60 | K2Ca(SO4)2:H2O |
| Tachyhydrite | -37.75 | -20.60 | 17.14 | Mg2CaCl6:12H2O |
| Thenardite | -6.12 | -6.48 | -0.36 | Na2SO4 |
| Thermonatrite | -10.43 | 0.50 | 10.94 | Na2CO3:H2O |
| Todorokite | -1.03 | -46.85 | -45.82 | Mn7O12:3H2O |
| Trona-K | -18.15 | -6.56 | 11.59 | K2NaH(CO3)2:2H2O |
| Zincite | -2.05 | 9.15 | 11.20 | ZnO |
| Zn | -50.60 | 18.19 | 68.79 | Zn |
| Zn(ClO4)2:6H2O | -117.80 | -112.16 | 5.63 | Zn(ClO4)2:6H2O |
| Zn(g) | -67.22 | 18.19 | 85.41 | Zn |
| Zn(OH)2(beta) | -2.78 | 9.15 | 11.93 | Zn(OH)2 |
| Zn(OH)2(epsilon) | -2.51 | 9.15 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -2.73 | 9.15 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -5.77 | 9.53 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -6.01 | 1.57 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -8.49 | 0.82 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -25.10 | -6.01 | 19.09 | Zn3O(SO4)2 |
| ZnCl2 | -15.49 | -8.41 | 7.08 | ZnCl2 |
| ZnCO3:H2O | -0.74 | -0.60 | 0.14 | ZnCO3:H2O |
| ZnSO4 | -11.11 | -7.58 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -5.88 | -7.58 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -5.71 | -7.58 | -1.88 | ZnSO4:7H2O |
| ZnSO4:H2O | -7.03 | -7.58 | -0.55 | ZnSO4:H2O |

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 2.

Mixture 2.

1.000e+000 Solution 1 Flujo 4
1.000e+000 Solution 3 AS2

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

| Elements | Molality | Moles |
|----------|------------|------------|
| Al | 4.752e-004 | 9.504e-004 |
| As | 3.445e-005 | 6.889e-005 |
| C | 1.262e-003 | 2.525e-003 |
| Ca | 5.496e-003 | 1.099e-002 |
| Cl | 1.025e-002 | 2.050e-002 |
| Cu | 2.767e-004 | 5.533e-004 |
| Fe | 1.526e-003 | 3.053e-003 |
| K | 1.408e-003 | 2.817e-003 |
| Mg | 6.902e-004 | 1.380e-003 |
| Mn | 1.888e-004 | 3.777e-004 |
| Na | 9.285e-003 | 1.857e-002 |
| S | 7.910e-003 | 1.582e-002 |
| Zn | 1.520e-004 | 3.039e-004 |

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

| | | | |
|--|---|---------------|-------------------------------|
| pH | = | 4.178 | Charge balance |
| pe | = | 10.602 | Adjusted to redox equilibrium |
| Activity of water | = | 0.999 | |
| Ionic strength | = | 3.618e-002 | |
| Mass of water (kg) | = | 2.000e+000 | |
| Total alkalinity (eq/kg) | = | -2.950e-004 | |
| Total CO2 (mol/kg) | = | 1.262e-003 | |
| Temperature (deg C) | = | 25.000 | |
| Electrical balance (eq) | = | 4.229e-003 | |
| Percent error, 100*(Cat- An)/(Cat+ An) | = | 4.52 | |
| Iterations | = | 18 | |
| Total H | = | 2.221065e+002 | |
| Total O | = | 1.111232e+002 | |

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

| Species | Molality | Activity | Log Molality | Log Activity | Log Gamma |
|----------------|------------|------------|--------------|--------------|-----------|
| H+ | 7.642e-005 | 6.645e-005 | -4.117 | -4.178 | -0.061 |
| OH- | 1.735e-010 | 1.449e-010 | -9.761 | -9.839 | -0.078 |
| H2O | 5.553e+001 | 9.994e-001 | 1.744 | -0.000 | 0.000 |
| Al | 4.752e-004 | | | | |
| Al+3 | 2.074e-004 | 5.731e-005 | -3.683 | -4.242 | -0.559 |
| AlSO4+ | 2.022e-004 | 1.696e-004 | -3.694 | -3.771 | -0.076 |
| Al(SO4)2- | 4.538e-005 | 3.807e-005 | -4.343 | -4.419 | -0.076 |
| AlOH+2 | 1.936e-005 | 9.656e-006 | -4.713 | -5.015 | -0.302 |
| Al(OH)2+ | 4.020e-007 | 3.372e-007 | -6.396 | -6.472 | -0.076 |
| Al2(OH)2+4 | 2.174e-007 | 1.516e-008 | -6.663 | -7.819 | -1.157 |
| Al3(OH)4+5 | 7.416e-009 | 1.269e-010 | -8.130 | -9.897 | -1.767 |
| HALO2 | 7.385e-009 | 7.385e-009 | -8.132 | -8.132 | 0.000 |
| AlO2- | 4.539e-011 | 3.807e-011 | -10.343 | -10.419 | -0.076 |
| NaAlO2 | 5.544e-014 | 5.544e-014 | -13.256 | -13.256 | 0.000 |
| Al13O4(OH)24+7 | 1.837e-017 | 6.305e-021 | -16.736 | -20.200 | -3.465 |
| As(-3) | 0.000e+000 | | | | |
| AsH3 | 0.000e+000 | 0.000e+000 | -110.165 | -110.165 | 0.000 |
| As(3) | 5.363e-017 | | | | |
| HAsO2 | 2.862e-017 | 2.862e-017 | -16.543 | -16.543 | 0.000 |
| As(OH)3 | 2.501e-017 | 2.501e-017 | -16.602 | -16.602 | 0.000 |
| H2AsO3- | 2.744e-022 | 2.302e-022 | -21.562 | -21.638 | -0.076 |
| AsO2- | 2.625e-022 | 2.202e-022 | -21.581 | -21.657 | -0.076 |
| AsO2OH-2 | 6.907e-029 | 3.385e-029 | -28.161 | -28.470 | -0.310 |
| HAsS2 | 0.000e+000 | 0.000e+000 | -186.171 | -186.171 | 0.000 |
| As(5) | 3.445e-005 | | | | |
| H2AsO4- | 3.397e-005 | 2.849e-005 | -4.469 | -4.545 | -0.076 |
| H3AsO4 | 3.335e-007 | 3.335e-007 | -6.477 | -6.477 | 0.000 |
| HAsO4-2 | 1.453e-007 | 7.118e-008 | -6.838 | -7.148 | -0.310 |
| AsO4-3 | 1.374e-014 | 2.748e-015 | -13.862 | -14.561 | -0.699 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -192.310 | -192.310 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -152.981 | -152.981 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -99.598 | -99.598 | 0.000 |
| C(2) | 3.172e-038 | | | | |
| CO | 3.172e-038 | 3.172e-038 | -37.499 | -37.499 | 0.000 |
| C(4) | 1.262e-003 | | | | |
| CO2 | 1.251e-003 | 1.262e-003 | -2.903 | -2.899 | 0.004 |
| HCO3- | 9.754e-006 | 8.182e-006 | -5.011 | -5.087 | -0.076 |
| FeHCO3+ | 1.443e-006 | 1.210e-006 | -5.841 | -5.917 | -0.076 |
| CaHCO3+ | 2.719e-007 | 2.280e-007 | -6.566 | -6.642 | -0.076 |
| NaHCO3 | 8.933e-008 | 8.933e-008 | -7.049 | -7.049 | 0.000 |
| FeCO3+ | 4.061e-008 | 3.406e-008 | -7.391 | -7.468 | -0.076 |
| MgHCO3+ | 3.018e-008 | 2.531e-008 | -7.520 | -7.597 | -0.076 |

| | | | | | |
|--------------|------------|------------|---------|---------|--------|
| ZnHCO3+ | 1.506e-008 | 1.263e-008 | -7.822 | -7.898 | -0.076 |
| CuCO3 | 5.537e-009 | 5.537e-009 | -8.257 | -8.257 | 0.000 |
| MnHCO3+ | 5.298e-009 | 4.444e-009 | -8.276 | -8.352 | -0.076 |
| FeCO3 | 8.741e-011 | 8.741e-011 | -10.058 | -10.058 | 0.000 |
| CaCO3 | 2.978e-011 | 2.978e-011 | -10.526 | -10.526 | 0.000 |
| MnCO3 | 1.364e-011 | 1.364e-011 | -10.865 | -10.865 | 0.000 |
| CO3-2 | 1.095e-011 | 5.463e-012 | -10.960 | -11.263 | -0.302 |
| ZnCO3 | 2.748e-012 | 2.748e-012 | -11.561 | -11.561 | 0.000 |
| MgCO3 | 1.539e-012 | 1.539e-012 | -11.813 | -11.813 | 0.000 |
| NaCO3- | 1.739e-013 | 1.459e-013 | -12.760 | -12.836 | -0.076 |
| Cu(CO3)2-2 | 1.100e-016 | 5.388e-017 | -15.959 | -16.269 | -0.310 |
| CuCO3(OH)2-2 | 2.173e-020 | 1.065e-020 | -19.663 | -19.973 | -0.310 |
| Ca | 5.496e-003 | | | | |
| Ca+2 | 4.497e-003 | 2.352e-003 | -2.347 | -2.629 | -0.281 |
| CaSO4 | 9.936e-004 | 9.936e-004 | -3.003 | -3.003 | 0.000 |
| CaCl+ | 5.049e-006 | 4.235e-006 | -5.297 | -5.373 | -0.076 |
| CaHCO3+ | 2.719e-007 | 2.280e-007 | -6.566 | -6.642 | -0.076 |
| CaCl2 | 4.232e-008 | 4.232e-008 | -7.373 | -7.373 | 0.000 |
| CaCO3 | 2.978e-011 | 2.978e-011 | -10.526 | -10.526 | 0.000 |
| CaOH+ | 5.957e-012 | 4.997e-012 | -11.225 | -11.301 | -0.076 |
| Cl(-1) | 1.025e-002 | | | | |
| Cl- | 1.022e-002 | 8.495e-003 | -1.990 | -2.071 | -0.080 |
| NaCl | 1.140e-005 | 1.140e-005 | -4.943 | -4.943 | 0.000 |
| CaCl+ | 5.049e-006 | 4.235e-006 | -5.297 | -5.373 | -0.076 |
| CuCl+ | 2.944e-006 | 2.470e-006 | -5.531 | -5.607 | -0.076 |
| MgCl+ | 2.106e-006 | 1.767e-006 | -5.677 | -5.753 | -0.076 |
| FeCl+ | 2.079e-006 | 1.744e-006 | -5.682 | -5.758 | -0.076 |
| MnCl+ | 1.538e-006 | 1.291e-006 | -5.813 | -5.889 | -0.076 |
| ZnCl+ | 1.019e-006 | 8.550e-007 | -5.992 | -6.068 | -0.076 |
| KCl | 3.262e-007 | 3.262e-007 | -6.486 | -6.486 | 0.000 |
| HCl | 1.268e-007 | 1.268e-007 | -6.897 | -6.897 | 0.000 |
| CaCl2 | 4.232e-008 | 4.232e-008 | -7.373 | -7.373 | 0.000 |
| FeCl2+ | 1.253e-008 | 1.051e-008 | -7.902 | -7.978 | -0.076 |
| CuCl2 | 1.105e-008 | 1.105e-008 | -7.957 | -7.957 | 0.000 |
| ZnCl2 | 8.485e-009 | 8.485e-009 | -8.071 | -8.071 | 0.000 |
| FeCl+2 | 3.065e-009 | 1.528e-009 | -8.514 | -8.816 | -0.302 |
| Zn(OH)Cl | 2.199e-010 | 2.199e-010 | -9.658 | -9.658 | 0.000 |
| FeCl2 | 7.951e-011 | 7.951e-011 | -10.100 | -10.100 | 0.000 |
| ZnCl3- | 4.745e-011 | 3.981e-011 | -10.324 | -10.400 | -0.076 |
| MnCl3- | 2.426e-011 | 2.035e-011 | -10.615 | -10.692 | -0.076 |
| CuCl2- | 8.299e-012 | 6.961e-012 | -11.081 | -11.157 | -0.076 |
| ZnCl4-2 | 5.231e-012 | 2.563e-012 | -11.281 | -11.591 | -0.310 |
| CuCl3-2 | 7.751e-013 | 3.798e-013 | -12.111 | -12.420 | -0.310 |
| FeCl4-2 | 3.384e-014 | 1.658e-014 | -13.471 | -13.780 | -0.310 |
| FeCl4- | 1.087e-015 | 9.121e-016 | -14.964 | -15.040 | -0.076 |
| CuCl4-2 | 3.054e-017 | 1.496e-017 | -16.515 | -16.825 | -0.310 |
| Cl(1) | 5.897e-028 | | | | |
| HClO | 5.894e-028 | 5.894e-028 | -27.230 | -27.230 | 0.000 |
| ClO- | 2.851e-031 | 2.392e-031 | -30.545 | -30.621 | -0.076 |
| Cl(3) | 0.000e+000 | | | | |
| ClO2- | 0.000e+000 | 0.000e+000 | -51.990 | -52.066 | -0.076 |
| HClO2 | 0.000e+000 | 0.000e+000 | -53.074 | -53.074 | 0.000 |
| Cl(5) | 0.000e+000 | | | | |
| ClO3- | 0.000e+000 | 0.000e+000 | -59.581 | -59.659 | -0.078 |
| Cl(7) | 0.000e+000 | | | | |
| ClO4- | 0.000e+000 | 0.000e+000 | -71.475 | -71.554 | -0.078 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -74.423 | -74.500 | -0.076 |
| Cu(1) | 1.081e-011 | | | | |
| CuCl2- | 8.299e-012 | 6.961e-012 | -11.081 | -11.157 | -0.076 |
| Cu+ | 1.736e-012 | 1.456e-012 | -11.761 | -11.837 | -0.076 |
| CuCl3-2 | 7.751e-013 | 3.798e-013 | -12.111 | -12.420 | -0.310 |
| Cu(2) | 2.767e-004 | | | | |
| Cu+2 | 2.032e-004 | 1.063e-004 | -3.692 | -3.974 | -0.281 |
| CuSO4 | 7.041e-005 | 7.041e-005 | -4.152 | -4.152 | 0.000 |
| CuCl+ | 2.944e-006 | 2.470e-006 | -5.531 | -5.607 | -0.076 |
| CuOH+ | 9.829e-008 | 8.245e-008 | -7.007 | -7.084 | -0.076 |
| CuCl2 | 1.105e-008 | 1.105e-008 | -7.957 | -7.957 | 0.000 |

| | | | | | |
|--------------|------------|------------|---------|---------|--------|
| CuCO3 | 5.537e-009 | 5.537e-009 | -8.257 | -8.257 | 0.000 |
| Cu(CO3)2-2 | 1.100e-016 | 5.388e-017 | -15.959 | -16.269 | -0.310 |
| CuCl4-2 | 3.054e-017 | 1.496e-017 | -16.515 | -16.825 | -0.310 |
| CuCO3(OH)2-2 | 2.173e-020 | 1.065e-020 | -19.663 | -19.973 | -0.310 |
| CuO2-2 | 3.945e-027 | 1.933e-027 | -26.404 | -26.714 | -0.310 |
| Fe(2) | 6.715e-004 | | | | |
| Fe+2 | 5.388e-004 | 2.818e-004 | -3.269 | -3.550 | -0.281 |
| FeSO4 | 1.292e-004 | 1.292e-004 | -3.889 | -3.889 | 0.000 |
| FeCl+ | 2.079e-006 | 1.744e-006 | -5.682 | -5.758 | -0.076 |
| FeHCO3+ | 1.443e-006 | 1.210e-006 | -5.841 | -5.917 | -0.076 |
| FeOH+ | 1.598e-009 | 1.340e-009 | -8.796 | -8.873 | -0.076 |
| FeCO3 | 8.741e-011 | 8.741e-011 | -10.058 | -10.058 | 0.000 |
| FeCl2 | 7.951e-011 | 7.951e-011 | -10.100 | -10.100 | 0.000 |
| FeCl4-2 | 3.384e-014 | 1.658e-014 | -13.471 | -13.780 | -0.310 |
| Fe(OH)2 | 1.601e-016 | 1.601e-016 | -15.796 | -15.796 | 0.000 |
| Fe(OH)3- | 1.143e-022 | 9.588e-023 | -21.942 | -22.018 | -0.076 |
| Fe(OH)4-2 | 2.943e-033 | 1.442e-033 | -32.531 | -32.841 | -0.310 |
| Fe(3) | 8.549e-004 | | | | |
| Fe(OH)2+ | 6.225e-004 | 5.222e-004 | -3.206 | -3.282 | -0.076 |
| FeOH+2 | 2.103e-004 | 1.049e-004 | -3.677 | -3.979 | -0.302 |
| Fe2(OH)2+4 | 4.244e-006 | 2.959e-007 | -5.372 | -6.529 | -1.157 |
| Fe+3 | 3.909e-006 | 1.080e-006 | -5.408 | -5.967 | -0.559 |
| Fe(OH)3 | 3.673e-006 | 3.673e-006 | -5.435 | -5.435 | 0.000 |
| Fe3(OH)4+5 | 1.887e-006 | 3.228e-008 | -5.724 | -7.491 | -1.767 |
| FeSO4+ | 3.602e-007 | 3.021e-007 | -6.444 | -6.520 | -0.076 |
| FeCO3+ | 4.061e-008 | 3.406e-008 | -7.391 | -7.468 | -0.076 |
| Fe(SO4)2- | 1.761e-008 | 1.477e-008 | -7.754 | -7.831 | -0.076 |
| FeCl2+ | 1.253e-008 | 1.051e-008 | -7.902 | -7.978 | -0.076 |
| FeCl+2 | 3.065e-009 | 1.528e-009 | -8.514 | -8.816 | -0.302 |
| Fe(OH)4- | 1.654e-011 | 1.388e-011 | -10.781 | -10.858 | -0.076 |
| FeCl4- | 1.087e-015 | 9.121e-016 | -14.964 | -15.040 | -0.076 |
| H(0) | 4.350e-033 | | | | |
| H2 | 2.175e-033 | 2.194e-033 | -32.663 | -32.659 | 0.004 |
| K | 1.408e-003 | | | | |
| K+ | 1.376e-003 | 1.144e-003 | -2.861 | -2.942 | -0.080 |
| KSO4- | 3.182e-005 | 2.669e-005 | -4.497 | -4.574 | -0.076 |
| KCl | 3.262e-007 | 3.262e-007 | -6.486 | -6.486 | 0.000 |
| KHSO4 | 1.565e-009 | 1.565e-009 | -8.806 | -8.806 | 0.000 |
| KOH | 5.964e-014 | 5.964e-014 | -13.224 | -13.224 | 0.000 |
| Mg | 6.902e-004 | | | | |
| Mg+2 | 4.824e-004 | 2.664e-004 | -3.317 | -3.575 | -0.258 |
| MgSO4 | 2.057e-004 | 2.057e-004 | -3.687 | -3.687 | 0.000 |
| MgCl+ | 2.106e-006 | 1.767e-006 | -5.677 | -5.753 | -0.076 |
| MgHCO3+ | 3.018e-008 | 2.531e-008 | -7.520 | -7.597 | -0.076 |
| MgCO3 | 1.539e-012 | 1.539e-012 | -11.813 | -11.813 | 0.000 |
| Mg4(OH)4+4 | 6.571e-037 | 4.581e-038 | -36.182 | -37.339 | -1.157 |
| Mn(2) | 1.888e-004 | | | | |
| Mn+2 | 1.364e-004 | 7.134e-005 | -3.865 | -4.147 | -0.281 |
| MnSO4 | 5.091e-005 | 5.091e-005 | -4.293 | -4.293 | 0.000 |
| MnCl+ | 1.538e-006 | 1.291e-006 | -5.813 | -5.889 | -0.076 |
| MnHCO3+ | 5.298e-009 | 4.444e-009 | -8.276 | -8.352 | -0.076 |
| MnOH+ | 3.288e-011 | 2.758e-011 | -10.483 | -10.559 | -0.076 |
| MnCl3- | 2.426e-011 | 2.035e-011 | -10.615 | -10.692 | -0.076 |
| MnCO3 | 1.364e-011 | 1.364e-011 | -10.865 | -10.865 | 0.000 |
| Mn2OH+3 | 9.759e-015 | 2.108e-015 | -14.011 | -14.676 | -0.665 |
| Mn(OH)2 | 1.018e-018 | 1.018e-018 | -17.992 | -17.992 | 0.000 |
| Mn2(OH)3+ | 2.599e-020 | 2.180e-020 | -19.585 | -19.662 | -0.076 |
| Mn(OH)3- | 1.713e-026 | 1.437e-026 | -25.766 | -25.843 | -0.076 |
| Mn(OH)4-2 | 3.734e-036 | 1.830e-036 | -35.428 | -35.738 | -0.310 |
| Mn(3) | 3.520e-019 | | | | |
| Mn+3 | 3.520e-019 | 7.604e-020 | -18.453 | -19.119 | -0.665 |
| Mn(6) | 0.000e+000 | | | | |
| MnO4-2 | 0.000e+000 | 0.000e+000 | -46.458 | -46.768 | -0.310 |
| Mn(7) | 0.000e+000 | | | | |
| MnO4- | 0.000e+000 | 0.000e+000 | -45.444 | -45.523 | -0.078 |
| Na | 9.285e-003 | | | | |
| Na+ | 9.100e-003 | 7.633e-003 | -2.041 | -2.117 | -0.076 |

| | | | | | |
|-----------|------------|------------|----------|----------|--------|
| NaSO4- | 1.739e-004 | 1.458e-004 | -3.760 | -3.836 | -0.076 |
| NaCl | 1.140e-005 | 1.140e-005 | -4.943 | -4.943 | 0.000 |
| NaHCO3 | 8.933e-008 | 8.933e-008 | -7.049 | -7.049 | 0.000 |
| NaOH | 1.908e-013 | 1.908e-013 | -12.719 | -12.719 | 0.000 |
| NaCO3- | 1.739e-013 | 1.459e-013 | -12.760 | -12.836 | -0.076 |
| NaAlO2 | 5.544e-014 | 5.544e-014 | -13.256 | -13.256 | 0.000 |
| O(0) | 2.619e-027 | | | | |
| O2 | 1.310e-027 | 1.321e-027 | -26.883 | -26.879 | 0.004 |
| S(-2) | 0.000e+000 | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -88.409 | -88.409 | 0.000 |
| HS- | 0.000e+000 | 0.000e+000 | -91.163 | -91.241 | -0.078 |
| S-2 | 0.000e+000 | 0.000e+000 | -99.694 | -99.989 | -0.295 |
| S2-2 | 0.000e+000 | 0.000e+000 | -162.354 | -162.663 | -0.310 |
| HAsS2 | 0.000e+000 | 0.000e+000 | -186.171 | -186.171 | 0.000 |
| S3-2 | 0.000e+000 | 0.000e+000 | -225.069 | -225.379 | -0.310 |
| S4-2 | 0.000e+000 | 0.000e+000 | -288.012 | -288.321 | -0.310 |
| S5-2 | 0.000e+000 | 0.000e+000 | -351.171 | -351.480 | -0.310 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -92.838 | -93.148 | -0.310 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -96.235 | -96.312 | -0.076 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -91.221 | -91.516 | -0.295 |
| S(4) | 2.618e-033 | | | | |
| HSO3- | 2.590e-033 | 2.172e-033 | -32.587 | -32.663 | -0.076 |
| H2SO3 | 1.384e-035 | 1.384e-035 | -34.859 | -34.859 | 0.000 |
| SO2 | 1.099e-035 | 1.099e-035 | -34.959 | -34.959 | 0.000 |
| SO3-2 | 3.846e-036 | 1.918e-036 | -35.415 | -35.717 | -0.302 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -51.052 | -51.362 | -0.310 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -116.250 | -116.560 | -0.310 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -165.543 | -165.852 | -0.310 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -243.714 | -244.024 | -0.310 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -69.846 | -70.156 | -0.310 |
| S(6) | 7.910e-003 | | | | |
| SO4-2 | 5.901e-003 | 2.892e-003 | -2.229 | -2.539 | -0.310 |
| CaSO4 | 9.936e-004 | 9.936e-004 | -3.003 | -3.003 | 0.000 |
| MgSO4 | 2.057e-004 | 2.057e-004 | -3.687 | -3.687 | 0.000 |
| AlSO4+ | 2.022e-004 | 1.696e-004 | -3.694 | -3.771 | -0.076 |
| NaSO4- | 1.739e-004 | 1.458e-004 | -3.760 | -3.836 | -0.076 |
| FeSO4 | 1.292e-004 | 1.292e-004 | -3.889 | -3.889 | 0.000 |
| CuSO4 | 7.041e-005 | 7.041e-005 | -4.152 | -4.152 | 0.000 |
| MnSO4 | 5.091e-005 | 5.091e-005 | -4.293 | -4.293 | 0.000 |
| Al(SO4)2- | 4.538e-005 | 3.807e-005 | -4.343 | -4.419 | -0.076 |
| ZnSO4 | 3.640e-005 | 3.640e-005 | -4.439 | -4.439 | 0.000 |
| KSO4- | 3.182e-005 | 2.669e-005 | -4.497 | -4.574 | -0.076 |
| HSO4- | 2.314e-005 | 1.941e-005 | -4.636 | -4.712 | -0.076 |
| FeSO4+ | 3.602e-007 | 3.021e-007 | -6.444 | -6.520 | -0.076 |
| Fe(SO4)2- | 1.761e-008 | 1.477e-008 | -7.754 | -7.831 | -0.076 |
| KHSO4 | 1.565e-009 | 1.565e-009 | -8.806 | -8.806 | 0.000 |
| H2SO4 | 1.217e-012 | 1.217e-012 | -11.915 | -11.915 | 0.000 |
| S(7) | 0.000e+000 | | | | |
| S2O8-2 | 0.000e+000 | 0.000e+000 | -49.017 | -49.327 | -0.310 |
| S(8) | 4.569e-038 | | | | |
| HSO5- | 4.569e-038 | 3.833e-038 | -37.340 | -37.417 | -0.076 |
| Zn | 1.520e-004 | | | | |
| Zn+2 | 1.145e-004 | 5.990e-005 | -3.941 | -4.223 | -0.281 |
| ZnSO4 | 3.640e-005 | 3.640e-005 | -4.439 | -4.439 | 0.000 |
| ZnCl+ | 1.019e-006 | 8.550e-007 | -5.992 | -6.068 | -0.076 |
| ZnHCO3+ | 1.506e-008 | 1.263e-008 | -7.822 | -7.898 | -0.076 |
| ZnCl2 | 8.485e-009 | 8.485e-009 | -8.071 | -8.071 | 0.000 |
| ZnOH+ | 1.178e-009 | 9.880e-010 | -8.929 | -9.005 | -0.076 |
| Zn(OH)Cl | 2.199e-010 | 2.199e-010 | -9.658 | -9.658 | 0.000 |
| ZnCl3- | 4.745e-011 | 3.981e-011 | -10.324 | -10.400 | -0.076 |
| ZnCl4-2 | 5.231e-012 | 2.563e-012 | -11.281 | -11.591 | -0.310 |
| ZnCO3 | 2.748e-012 | 2.748e-012 | -11.561 | -11.561 | 0.000 |
| Zn(OH)2 | 6.364e-014 | 6.364e-014 | -13.196 | -13.196 | 0.000 |
| Zn(OH)3- | 3.537e-021 | 2.967e-021 | -20.451 | -20.528 | -0.076 |

| | | | | | |
|-----------|------------|------------|---------|---------|--------|
| Zn(OH)4-2 | 1.552e-029 | 7.608e-030 | -28.809 | -29.119 | -0.310 |
| ZnClO4+ | 0.000e+000 | 0.000e+000 | -74.423 | -74.500 | -0.076 |

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

| Phase | SI | log IAP | log KT | |
|--------------------|---------|---------|---------|-------------------|
| Al | -121.46 | 28.45 | 149.91 | Al |
| Al(g) | -172.17 | 28.45 | 200.62 | Al |
| Al2(SO4)3 | -35.00 | -16.10 | 18.90 | Al2(SO4)3 |
| Al2(SO4)3:6H2O | -17.66 | -16.10 | 1.56 | Al2(SO4)3:6H2O |
| Alabandite | -90.79 | -91.21 | -0.42 | MnS |
| Alum-K | -7.29 | -12.26 | -4.97 | KAl(SO4)2:12H2O |
| Alunite | 4.79 | 4.32 | -0.47 | KAl3(OH)6(SO4)2 |
| Anhydrite | -0.82 | -5.17 | -4.35 | CaSO4 |
| Antarcticite | -10.87 | -6.77 | 4.09 | CaCl2:6H2O |
| Antlerite | -6.48 | 2.25 | 8.73 | Cu3(SO4)(OH)4 |
| Aphthitalite | -12.13 | -16.02 | -3.89 | NaK3(SO4)2 |
| Aragonite | -5.51 | -3.54 | 1.97 | CaCO3 |
| Arcanite | -6.58 | -8.42 | -1.84 | K2SO4 |
| Arsenolite | -31.79 | -51.63 | -19.84 | As2O3 |
| Arsenopyrite | -144.16 | -158.60 | -14.45 | FeAsS |
| Artinite | -19.33 | 0.30 | 19.63 | Mg2CO3(OH)2:3H2O |
| As | -48.34 | -5.66 | 42.68 | As |
| As2O5 | -19.58 | -17.44 | 2.14 | As2O5 |
| As4O6(cubi) | -63.44 | -103.26 | -39.82 | As4O6 |
| As4O6(mono) | -63.21 | -103.26 | -40.05 | As4O6 |
| Atacamite | -9.24 | 5.03 | 14.26 | Cu4Cl2(OH)6 |
| Azurite | -14.50 | -5.39 | 9.12 | Cu3(CO3)2(OH)2 |
| Bassanite | -1.46 | -5.17 | -3.71 | CaSO4:0.5H2O |
| Birnessite | -58.78 | -144.33 | -85.55 | Mn8O14:5H2O |
| Bischofite | -12.11 | -7.72 | 4.39 | MgCl2:6H2O |
| Bixbyite | -12.21 | -13.17 | -0.96 | Mn2O3 |
| Bloedite | -10.41 | -12.89 | -2.48 | Na2Mg(SO4)2:4H2O |
| Boehmite | 0.74 | 8.29 | 7.55 | AlO2H |
| Bornite | -300.59 | -403.12 | -102.53 | Cu5FeS4 |
| Brochantite | -8.79 | 6.63 | 15.42 | Cu4(SO4)(OH)6 |
| Brucite | -11.50 | 4.78 | 16.28 | Mg(OH)2 |
| Burkeite | -28.18 | -18.69 | 9.49 | Na6CO3(SO4)2 |
| C | -46.53 | 17.61 | 64.15 | C |
| C(g) | -164.15 | 17.61 | 181.77 | C |
| Ca | -120.67 | 19.17 | 139.83 | Ca |
| Ca(g) | -145.91 | 19.17 | 165.07 | Ca |
| Ca2Al2O5:8H2O | -31.54 | 28.03 | 59.57 | Ca2Al2O5:8H2O |
| Ca2Cl2(OH)2:H2O | -27.33 | -1.04 | 26.29 | Ca2Cl2(OH)2:H2O |
| Ca3(AsO4)2 | -18.07 | -0.27 | 17.80 | Ca3(AsO4)2 |
| Ca3Al2O6 | -79.27 | 33.76 | 113.03 | Ca3Al2O6 |
| Ca4Al2Fe2O10 | -87.87 | 52.62 | 140.48 | Ca4Al2Fe2O10 |
| Ca4Al2O7:13H2O | -67.77 | 39.48 | 107.25 | Ca4Al2O7:13H2O |
| Ca4Al2O7:19H2O | -64.20 | 39.48 | 103.68 | Ca4Al2O7:19H2O |
| Ca4Cl2(OH)6:13H2O | -57.92 | 10.40 | 68.33 | Ca4Cl2(OH)6:13H2O |
| CaAl2O4 | -24.60 | 22.31 | 46.91 | CaAl2O4 |
| CaAl2O4:10H2O | -15.69 | 22.30 | 37.99 | CaAl2O4:10H2O |
| CaAl4O7 | -29.70 | 38.89 | 68.59 | CaAl4O7 |
| Calcite | -5.36 | -3.54 | 1.82 | CaCO3 |
| Carnallite | -17.00 | -12.73 | 4.27 | KMgCl3:6H2O |
| CaSO4:0.5H2O(beta) | -1.63 | -5.17 | -3.54 | CaSO4:0.5H2O |
| CH4(g) | -96.76 | -99.60 | -2.84 | CH4 |
| Chalcanthite | -3.88 | -6.51 | -2.63 | CuSO4:5H2O |
| Chalcocite | -75.99 | -110.74 | -34.74 | Cu2S |
| Chalcocyanite | -9.42 | -6.51 | 2.91 | CuSO4 |
| Chalcopyrite | -149.05 | -181.65 | -32.60 | CuFeS2 |
| Chloromagnesite | -29.53 | -7.72 | 21.82 | MgCl2 |
| Cl2(g) | -28.93 | -25.94 | 2.99 | Cl2 |
| Claudetite | -31.83 | -51.63 | -19.80 | As2O3 |
| CO(g) | -34.50 | -37.50 | -3.00 | CO |
| CO2(g) | -1.44 | -9.26 | -7.83 | CO2 |

| | | | | |
|--|--------|--------|--------|--|
| Corundum | -1.71 | 16.58 | 18.29 | Al ₂ O ₃ |
| Covellite | -68.18 | -91.04 | -22.86 | CuS |
| Cu | -13.68 | 17.82 | 31.50 | Cu |
| Cu(g) | -65.83 | 17.82 | 83.66 | Cu |
| CuCl ₂ | -11.84 | -8.12 | 3.72 | CuCl ₂ |
| Cuprite | -13.41 | -15.32 | -1.91 | Cu ₂ O |
| Dawsonite | -3.26 | 1.09 | 4.34 | NaAlCO ₃ (OH) ₂ |
| Delafossite | 5.34 | -1.09 | -6.44 | CuFeO ₂ |
| Diaspore | 1.14 | 8.29 | 7.15 | AlHO ₂ |
| Dolomite | -10.50 | -8.02 | 2.47 | CaMg(CO ₃) ₂ |
| Dolomite-dis | -12.03 | -8.02 | 4.01 | CaMg(CO ₃) ₂ |
| Dolomite-ord | -10.49 | -8.02 | 2.46 | CaMg(CO ₃) ₂ |
| Epsomite | -4.15 | -6.12 | -1.96 | MgSO ₄ ·7H ₂ O |
| Ettringite | -44.22 | 18.25 | 62.46 | Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ ·26H ₂ O |
| Fe | -40.77 | 18.24 | 59.02 | Fe |
| Fe(OH) ₂ | -9.09 | 4.80 | 13.89 | Fe(OH) ₂ |
| Fe(OH) ₃ | 0.93 | 6.57 | 5.64 | Fe(OH) ₃ |
| Fe ₂ (SO ₄) ₃ | -22.60 | -19.55 | 3.05 | Fe ₂ (SO ₄) ₃ |
| FeO | -8.72 | 4.80 | 13.52 | FeO |
| Ferrite-Ca | -2.64 | 18.86 | 21.50 | CaFe ₂ O ₄ |
| Ferrite-Cu | 7.23 | 17.51 | 10.28 | CuFe ₂ O ₄ |
| Ferrite-Dicalcium | -32.22 | 24.58 | 56.80 | Ca ₂ Fe ₂ O ₅ |
| Ferrite-Mg | -3.11 | 17.91 | 21.02 | MgFe ₂ O ₄ |
| Ferrite-Zn | 5.56 | 17.26 | 11.70 | ZnFe ₂ O ₄ |
| FeSO ₄ | -8.70 | -6.09 | 2.61 | FeSO ₄ |
| Gaylussite | -19.85 | -8.68 | 11.16 | CaNa ₂ (CO ₃) ₂ ·5H ₂ O |
| Gibbsite | 0.55 | 8.29 | 7.74 | Al(OH) ₃ |
| Glauberite | -6.47 | -11.94 | -5.47 | Na ₂ Ca(SO ₄) ₂ |
| Goethite | 6.04 | 6.57 | 0.53 | FeOOH |
| Gypsum | -0.64 | -5.17 | -4.53 | CaSO ₄ ·2H ₂ O |
| H ₂ (g) | -29.56 | -32.66 | -3.10 | H ₂ |
| H ₂ O(g) | -1.59 | -0.00 | 1.59 | H ₂ O |
| H ₂ S(g) | -87.43 | -95.42 | -7.99 | H ₂ S |
| Halite | -5.75 | -4.19 | 1.56 | NaCl |
| Hausmannite | -19.11 | -8.97 | 10.14 | Mn ₃ O ₄ |
| HCl(g) | -12.55 | -6.25 | 6.30 | HCl |
| Hematite | 13.06 | 13.13 | 0.08 | Fe ₂ O ₃ |
| Hercynite | -7.42 | 21.39 | 28.80 | FeAl ₂ O ₄ |
| Hexahydrite | -4.39 | -6.11 | -1.73 | MgSO ₄ ·6H ₂ O |
| Huntite | -27.21 | -16.99 | 10.22 | CaMg ₃ (CO ₃) ₄ |
| Hydromagnesite | -43.90 | -13.16 | 30.74 | Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O |
| Hydrophilite | -18.52 | -6.77 | 11.75 | CaCl ₂ |
| Hydrozincite | -28.18 | 2.13 | 30.31 | Zn ₅ (OH) ₆ (CO ₃) ₂ |
| Ice | -0.14 | -0.00 | 0.14 | H ₂ O |
| Jarosite | 8.55 | -0.86 | -9.41 | KFe ₃ (SO ₄) ₂ (OH) ₆ |
| Jarosite-Na | 5.42 | -0.03 | -5.45 | NaFe ₃ (SO ₄) ₂ (OH) ₆ |
| K | -63.02 | 7.96 | 70.98 | K |
| K(g) | -73.62 | 7.96 | 81.58 | K |
| K ₂ CO ₃ ·1.5H ₂ O | -20.17 | -6.79 | 13.38 | K ₂ CO ₃ ·1.5H ₂ O |
| K ₂ O | -81.56 | 2.47 | 84.04 | K ₂ O |
| K ₃ H(SO ₄) ₂ | -14.46 | -18.08 | -3.62 | K ₃ H(SO ₄) ₂ |
| K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O | -73.41 | -45.70 | 27.71 | K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O |
| Kainite | -10.82 | -11.13 | -0.31 | KMgClSO ₄ ·3H ₂ O |
| KAl(SO ₄) ₂ | -15.53 | -12.26 | 3.27 | KAl(SO ₄) ₂ |
| Kalinite | -8.31 | -8.03 | 0.28 | KHCO ₃ |
| Katoite | -45.19 | 33.76 | 78.94 | Ca ₃ Al ₂ H ₁₂ O ₁₂ |
| Kieserite | -5.85 | -6.11 | -0.27 | MgSO ₄ ·H ₂ O |
| KMgCl ₃ | -33.98 | -12.73 | 21.25 | KMgCl ₃ |
| KMgCl ₃ ·2H ₂ O | -26.69 | -12.73 | 13.96 | KMgCl ₃ ·2H ₂ O |
| KNaCO ₃ ·6H ₂ O | -16.23 | -5.97 | 10.26 | KNaCO ₃ ·6H ₂ O |
| Lammerite | -5.86 | -4.30 | 1.55 | Cu ₃ (AsO ₄) ₂ |
| Lansfordite | -9.33 | -4.49 | 4.84 | MgCO ₃ ·5H ₂ O |
| Lawrencite | -16.75 | -7.69 | 9.05 | FeCl ₂ |
| Leonite | -10.42 | -14.54 | -4.11 | K ₂ Mg(SO ₄) ₂ ·4H ₂ O |
| Lime | -26.84 | 5.73 | 32.57 | CaO |
| Magnesite | -6.76 | -4.48 | 2.27 | MgCO ₃ |
| Magnetite | 7.52 | 17.94 | 10.42 | Fe ₃ O ₄ |

| | | | | |
|--|---------|---------|--------|---|
| Malachite | -6.40 | -0.50 | 5.90 | Cu ₂ CO ₃ (OH) ₂ |
| Manganite | -6.42 | -6.59 | -0.16 | MnO(OH) |
| Manganosite | -13.71 | 4.21 | 17.92 | MnO |
| Mayenite | -309.37 | 184.78 | 494.15 | Ca ₁₂ Al ₁₄ O ₃₃ |
| Melanterite | -3.69 | -6.09 | -2.40 | FeSO ₄ ·7H ₂ O |
| Mercallite | -8.22 | -9.66 | -1.44 | KHSO ₄ |
| Mg | -104.30 | 18.22 | 122.52 | Mg |
| Mg(g) | -124.03 | 18.22 | 142.25 | Mg |
| Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O | -10.11 | -4.92 | 5.20 | Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O |
| Mg _{1.5} SO ₄ (OH) | -12.93 | -3.72 | 9.21 | Mg _{1.5} SO ₄ (OH) |
| MgCl ₂ :2H ₂ O | -20.45 | -7.72 | 12.73 | MgCl ₂ :2H ₂ O |
| MgCl ₂ :4H ₂ O | -15.02 | -7.72 | 7.30 | MgCl ₂ :4H ₂ O |
| MgCl ₂ :H ₂ O | -23.79 | -7.72 | 16.07 | MgCl ₂ :H ₂ O |
| MgOHCl | -17.36 | -1.47 | 15.89 | MgOHCl |
| MgSO ₄ | -10.94 | -6.11 | 4.83 | MgSO ₄ |
| Mirabilite | -5.62 | -6.78 | -1.15 | Na ₂ SO ₄ :10H ₂ O |
| Misenite | -55.30 | -66.37 | -11.08 | K ₈ H ₆ (SO ₄) ₇ |
| Mn | -65.29 | 17.65 | 82.93 | Mn |
| Mn(OH) ₂ (am) | -11.10 | 4.21 | 15.31 | Mn(OH) ₂ |
| Mn(OH) ₃ | -12.93 | -6.59 | 6.34 | Mn(OH) ₃ |
| MnCl ₂ :2H ₂ O | -12.29 | -8.29 | 4.00 | MnCl ₂ :2H ₂ O |
| MnCl ₂ :4H ₂ O | -11.04 | -8.29 | 2.75 | MnCl ₂ :4H ₂ O |
| MnCl ₂ :H ₂ O | -13.83 | -8.29 | 5.54 | MnCl ₂ :H ₂ O |
| MnO ₂ (gamma) | -9.33 | -25.46 | -16.13 | MnO ₂ |
| MnSO ₄ | -9.29 | -6.69 | 2.61 | MnSO ₄ |
| Molysite | -25.65 | -12.18 | 13.47 | FeCl ₃ |
| Monohydrocalcite | -6.22 | -3.54 | 2.68 | CaCO ₃ :H ₂ O |
| Na | -58.59 | 8.78 | 67.37 | Na |
| Na(g) | -72.08 | 8.78 | 80.86 | Na |
| Na ₂ CO ₃ | -16.31 | -5.14 | 11.16 | Na ₂ CO ₃ |
| Na ₂ CO ₃ :7H ₂ O | -15.08 | -5.15 | 9.94 | Na ₂ CO ₃ :7H ₂ O |
| Na ₂ O | -63.30 | 4.12 | 67.42 | Na ₂ O |
| Na ₃ H(SO ₄) ₂ | -14.72 | -15.61 | -0.89 | Na ₃ H(SO ₄) ₂ |
| Na ₄ Ca(SO ₄) ₃ :2H ₂ O | -12.82 | -18.71 | -5.89 | Na ₄ Ca(SO ₄) ₃ :2H ₂ O |
| NaFeO ₂ | -11.26 | 8.63 | 19.88 | NaFeO ₂ |
| Nahcolite | -7.06 | -7.20 | -0.14 | NaHCO ₃ |
| Nantokite | -7.14 | -13.91 | -6.77 | CuCl |
| Natron | -14.74 | -5.15 | 9.59 | Na ₂ CO ₃ :10H ₂ O |
| Nesquehonite | -9.77 | -4.48 | 5.29 | MgCO ₃ :3H ₂ O |
| O ₂ (g) | -23.99 | -26.88 | -2.89 | O ₂ |
| Orpiment | -258.40 | -337.88 | -79.49 | As ₂ S ₃ |
| Oxychloride-Mg | -22.52 | 3.31 | 25.83 | Mg ₂ Cl(OH) ₃ :4H ₂ O |
| Pentahydrite | -4.73 | -6.11 | -1.39 | MgSO ₄ :5H ₂ O |
| Periclase | -16.54 | 4.78 | 21.33 | MgO |
| Picromerite | -10.10 | -14.54 | -4.44 | K ₂ Mg(SO ₄) ₂ :6H ₂ O |
| Pirssonite | -20.01 | -8.68 | 11.32 | Na ₂ Ca(CO ₃) ₂ :2H ₂ O |
| Polyhalite | -10.56 | -24.87 | -14.31 | K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O |
| Portlandite | -16.82 | 5.73 | 22.55 | Ca(OH) ₂ |
| Pyrite | -140.20 | -164.90 | -24.70 | FeS ₂ |
| Pyrolusite | -7.80 | -25.46 | -17.66 | MnO ₂ |
| Pyrrhotite | -86.87 | -90.61 | -3.74 | FeS |
| Realgar | -99.82 | -160.10 | -60.28 | AsS |
| Rhodochrosite | -4.84 | -5.06 | -0.22 | MnCO ₃ |
| S | -63.75 | -108.86 | -45.11 | S |
| S ₂ (g) | -141.39 | -148.57 | -7.19 | S ₂ |
| Scacchite | -17.03 | -8.29 | 8.74 | MnCl ₂ |
| Siderite | -4.24 | -4.46 | -0.22 | FeCO ₃ |
| Smithsonite | -5.58 | -5.13 | 0.44 | ZnCO ₃ |
| SO ₂ (g) | -35.13 | -34.96 | 0.18 | SO ₂ |
| Sphalerite | -79.82 | -91.29 | -11.47 | ZnS |
| Spinel | -16.24 | 21.36 | 37.61 | Al ₂ MgO ₄ |
| Starkeyite | -5.11 | -6.11 | -1.00 | MgSO ₄ :4H ₂ O |
| Sylvite | -5.84 | -5.01 | 0.83 | KCl |
| Syngenite | -5.99 | -13.59 | -7.60 | K ₂ Ca(SO ₄) ₂ :H ₂ O |
| Tachyhydrite | -39.35 | -22.21 | 17.14 | Mg ₂ CaCl ₆ :12H ₂ O |
| Tenorite | -3.27 | 4.38 | 7.65 | CuO |
| Thenardite | -6.42 | -6.77 | -0.36 | Na ₂ SO ₄ |

| | | | | |
|------------------|---------|---------|--------|------------------|
| Thermonatrite | -16.08 | -5.14 | 10.94 | Na2CO3:H2O |
| Todorokite | -48.82 | -94.64 | -45.82 | Mn7O12:3H2O |
| Troilite | -86.77 | -90.61 | -3.84 | FeS |
| Trona-K | -25.59 | -14.00 | 11.59 | K2NaH(CO3)2:2H2O |
| Wurtzite | -82.12 | -91.29 | -9.17 | ZnS |
| Wustite | -7.67 | 4.74 | 12.40 | Fe.9470 |
| Zincite | -7.07 | 4.13 | 11.20 | ZnO |
| Zn | -51.22 | 17.57 | 68.79 | Zn |
| Zn(ClO4)2:6H2O | -152.97 | -147.33 | 5.63 | Zn(ClO4)2:6H2O |
| Zn(g) | -67.84 | 17.57 | 85.41 | Zn |
| Zn(OH)2(beta) | -7.80 | 4.13 | 11.93 | Zn(OH)2 |
| Zn(OH)2(epsilon) | -7.53 | 4.13 | 11.66 | Zn(OH)2 |
| Zn(OH)2(gamma) | -7.75 | 4.13 | 11.88 | Zn(OH)2 |
| Zn2(OH)3Cl | -13.28 | 2.02 | 15.29 | Zn2(OH)3Cl |
| Zn2SO4(OH)2 | -10.21 | -2.63 | 7.58 | Zn2SO4(OH)2 |
| Zn3(AsO4)2 | -14.36 | -5.05 | 9.31 | Zn3(AsO4)2 |
| Zn3O(SO4)2 | -28.48 | -9.39 | 19.09 | Zn3O(SO4)2 |
| ZnCl2 | -15.44 | -8.36 | 7.08 | ZnCl2 |
| ZnCO3:H2O | -5.27 | -5.13 | 0.14 | ZnCO3:H2O |
| ZnSO4 | -10.29 | -6.76 | 3.53 | ZnSO4 |
| ZnSO4:6H2O | -5.06 | -6.76 | -1.70 | ZnSO4:6H2O |
| ZnSO4:7H2O | -4.89 | -6.76 | -1.88 | ZnSO4:7H2O |
| ZnSO4:H2O | -6.21 | -6.76 | -0.55 | ZnSO4:H2O |

End of simulation.

Reading input data for simulation 2.

End of run.
