Table DR1 with comments (11 pages)

Species and sources of thermodynamic data for parts of the chemical system Na-K-Al-Si-Fe-Au-Cl-S-O-H at 500 bar and 25–400 °C, with comments about thermodynamic modelling approach and software

1. Comments about modelling software and assumption for this GEOLOGY paper

Calculations using the multicomponent heterogeneous equilibrium speciation code CHEMIX (Turnbull and Wadsley, 1986; extended by additional data formats and an Excel frontend programmed by X. Liu and V. Pokrovskii at ETH Zürich) assumed single-step transfer of the model fluid composition to conditions of 500 bar and variable temperatures between 450 and 200°C. Mineral phases in the chosen subssystem (notably pyrite, native sulfur and alunite as well as Na-K-Al silicate minerals) are allowed to precipitate and account for the decrease in total sulfur content in the fluid with decreasing temperature shown in Figure 2. A more extensive study, including aqueous Cu and As species and other reaction scenarios, is in preparation and shows that additional precipitation of Cu-Fe-sulfide further accentuates the pivotal effects of the mass balance between Fe+Cu and S upon Au transport.

Computations shown in this paper were restricted to a segment of isobaric cooling at 500bar because thermodynamic data are most reliable at this pressure, for the most important cooling interval between 450°C and 300°C after the contracting vapour crosses above the critical curve. No precise thermodynamic data are available for higher temperatures, but fluid inclusion analyses by Ulrich et al. (2001) for Bajo de la Alumbrera and unpublished data for the Bingham porphyry-Cu-Au deposit indicate that little or no gold and sulfide precipitation occurs above 450°C, in agreement with published thermodynamic estimates (Hezarkhani et al., 1999). Additional thermodynamic data by Stefánsson and Seward (2003, 2004) for T<350°C and the vapor saturation pressure show that gold solubility is not significantly pressure dependent once the decisive cooling interval from 450 to 300°C has been passed. The thermodynamic computations are therefore approximately valid for any *P-T* path within the isocompositional plane marked by multiple arrows in Figure 1. Starting compositions determined by processes above 450°C / 500bar, although still poorly constrained by experimental data, are decisive for the subsequent fluid evolution, as shown by the three modeling scenarios presented in Figure 2 and discussed in the text of the paper.

Activity coefficients for solute species in the aqueous phase were calculated according to equations by Oelkers and Helgeson (1991) using parameters consistent with gold solubility data interpretation by Stefansson (2003).

2. Species list and data sources

Species	Data Source
Gases	
$S_2(g)$	Turnbull and Wadsley (1986) CPDMRL
$H_2(g)$	Turnbull and Wadsley (1986) CPDMRL
$H_2O(g)$	Turnbull and Wadsley, 1986) CPDMRL
$H_2S(g)$	Turnbull and Wadsley, 1986) CPDMRL
$N_2(g)$	Turnbull and Wadsley, 1986) CPDMRL
Aqueous species	
H_2O liquid	Johnson et al. (1992)
$OH^-(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$H_2(aq)$	Stefansson (2003)
HCl(aq)	Ho et al., (2001) as used by Stefansson (2003)
$H^+(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
NaCl(aq)	Johnson et al. (1992), update Sverjensky et al. (1997)
$Na^+(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
NaOH(aq)	Johnson et al. (1992), update Sverjensky et al. (1997)
KCl(aq)	Johnson et al. (1992), update Sverjensky et al. (1997)
$K^+(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$Cl^-(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$FeCl_2(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$FeCl^+(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$Fe^{2+}(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$H_2S(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$HS^-(aq)$	Stefansson (2003)
NaHS(aq)	Stefansson (2003)
$SO_2(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$HSO_3^-(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$SO_3^{2-}(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$HSO_4^-(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$NaSO_4^-(aq)$	Estimated from SUPCRT95 (Johnson et al., 1992) assuming $NaSO_4^-(aq)=KSO_4^-(aq)–NaCl(aq)+KCl(aq)$
$KSO_4^-(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$SO_4^{2-}(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
$SiO_2(aq)$	Johnson et al. (1992), update Sverjensky et al. (1997)
AuHS(aq)	Stefansson (2003)
$Au(HS)_2^-(aq)$	Stefansson (2003)
$AuCl_2^-(aq)$	Stefansson (2003)
AuOH(aq)	Stefansson (2003)

Species list and data sources (Continued)

Species	Abbreviation	Data Source
Solids		
$KAlSi_3O_8$	ksp	Johnson et al. (1992)
$NaAlSi_3O_8$	ab	Johnson et al. (1992)
$KAl_3Si_3O_{10}(OH)_2$	mus	Johnson et al. (1992)
$Al_2Si_2O_5(OH)_4$	kao	Johnson et al. (1992)
$Al_2Si_4O_{10}(OH)_2$	pyp	Johnson et al. (1992)
Al_2SiO_5	and	Johnson et al. (1992)
SiO_2	qz	Johnson et al. (1992)
AlOOH	dsp	Johnson et al. (1992)
FeS_2	py	Johnson et al. (1992)
FeS	po	Johnson et al. (1992)
Fe_3O_4	mt	Johnson et al. (1992)
Fe_2O_3	hem	Johnson et al. (1992)
Au	gold	Turnbull and Wadsley (1986) CPDMRL
S	S	Turnbull and Wadsley (1986) CPDMRL

Full data set is listed below, consistent with the ETH-modified CSIRO-THERMODATA software package (Turnbull and Wadsley, 1986; Heinrich et al., 1996; Pokrovskii, unpubl.).

3. Additional references for Repository

Ho, P.C., Palmer, D.A. and Gruszkiewicz, M.S., 2001. Conductivity measurements of dilute aqueous HCl solutions to high temperatures and pressures using a flow-through cell. Journal of Physical Chemistry B, 105(6): 1260-1266.

Heinrich, C.A., Walshe, J.L. and Harrold, B.P., 1996. Chemical mass transfer modelling of ore-forming hydrothermal systems: Current practise and problems. Ore Geology Reviews, 10(3-6): 319-338.

Herzarkhani, A., Williams-Jones, A.E., and Gammons, C.H., 1999, Factors controlling copper solubility and chalcopyrite deposition in the Sungun porphyry copper deposit, Iran: Mineralium Deposita, v. 34, p. 770-783.

Johnson, J.W., Oelkers, E.H. and Helgeson, H.C., 1992. SUPCTR92 - a Software Package for Calculating the Standard Molal Thermodynamic Properties of Minerals, Gases, Aqueous Species, and Reactions from 1 bar to 5000 bar and 0°C to 1000°C. Computers & Geosciences, 18(7): 899-947.

Oelkers, E.H. and Helgeson, H.C., 1991. Calculation of Activity-Coefficients and Degrees of Formation of Neutral Ion-Pairs in Supercritical Electrolyte-Solutions. Geochimica Et Cosmochimica Acta, 55(5): 1235-1251.

Stefánsson, A., 2003. The stability and stoichiometry of gold(I) and silver(I) complexes in hydrothermal solutions. PhD Thesis 14808, ETH Zürich: 142 p., 2 Appendices.

Sverjensky, D.A., Shock, E.L. and Helgeson, H.C., 1997. Prediction of the thermodynamic properties of aqueous metal complexes to 1000 degrees C and 5 kb. Geochimica Et Cosmochimica Acta, 61(7): 1359-1412.

Turnbull, A.G. and Wadsley, M.W., 1986. The CSIRO - SGTE THERMODATA System (Version V). Commonwealth Scientific and Industrial Research Organisation, Port Melbourne, Division of Mineral Chemistry Communications, 1-7: 413.

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4. Full thermodynamic data in CSIRO-THERMODATA format

Data type formats “GIB”, “CPD” and “ETH” according to ETH-modified version by V. Pokrovskii (ETH Zürich, 1999). CuAuAs-Dataset version 12. September, searching in sequence GIB500 CPDCH03 ETHMIN95 ETHCH03 ETHAQU95 CPDMRL.
All units in mol, cal, bar and K (temperature limits in °C).
Data type GIB lists fit parameters a, b, c, d, e and f referring to
DfG (500 bar) = a + b*T + c*T*T + d*T*T*T + e/T + f*T*ln(T) in cal/mol, where T is the temperature in K

```
H2 (G)                                  Source CPDMRL        Data type CPD
hydrogen diatomic gas
DfH = 0.000000 cal/mol  S = 31.2070 cal/K/mol
Cp = 7.18062 + (-.592740E-03*T) + (0.641294E-06*T*T) + (-14285.2/T/T)
Tmax = 1226.85 C      DtrH = 0.000000 cal/mol
Cp = 7.46736 + (0.580198E-03*T) + (-.226250E-07*T*T) + (-.132201E+07/T/T)
Tmax = 5726.85 C      DtrH = 0.000000 cal/mol

S2 (g)                                  Source CPDMRL        Data type CPD
sulfur gas diatomic
DfH = 30840.0 cal/mol  S = 54.5100 cal/K/mol
Cp = 7.55235 + (0.275658E-02*T) + (-.149540E-05*T*T) + (-42965.1/T/T)
Tmax = 526.850 C      DtrH = 0.000000 cal/mol
Cp = 8.92992 + (0.686544E-04*T) + (-.532360E-09*T*T) + (-161047./T/T)
Tmax = 5726.85 C      DtrH = 0.000000 cal/mol

H2O (G)                                 Source CPDMRL        Data type CPD
hydrogen oxide gas water steam
DfH = -57798.0 cal/mol  S = 45.1060 cal/K/mol
Cp = 6.92691 + (0.264398E-02*T) + (0.255648E-06*T*T) + (25572.3/T/T)
Tmax = 726.850 C      DtrH = 0.000000 cal/mol
Cp = 5.81776 + (0.484525E-02*T) + (-.823864E-06*T*T) + (0.000000/T/T)
Tmax = 1726.85 C      DtrH = 0.000000 cal/mol

H2S (g)                                 Source CPDMRL        Data type CPD
hydrogen sulfide gas
DfH = -4880.00 cal/mol  S = 49.1510 cal/K/mol
Cp = 7.81000 + (0.296000E-02*T) + (0.000000*T*T) + (-46000.0/T/T)
Tmax = 2026.85 C      DtrH = 0.000000 cal/mol

N2 (g)                                  Source CPDMRL        Data type CPD
nitrogen diatomic gas
DfH = 0.000000 cal/mol  S = 45.7700 cal/K/mol
Cp = 6.51773 + (0.560719E-03*T) + (0.811435E-06*T*T) + (18257.7/T/T)
Tmax = 526.850 C      DtrH = 0.000000 cal/mol
Cp = 6.57285 + (0.177454E-02*T) + (-.371390E-06*T*T) + (-157601./T/T)
Tmax = 1726.85 C      DtrH = 0.000000 cal/mol
Cp = 8.92185 + (0.228148E-04*T) + (0.405211E-08*T*T) + (-.154282E+07/T/T)
Tmax = 5726.85 C      DtrH = 0.000000 cal/mol

H2 O (AQ)                               Source ETHAQU95      Data type ETH

Parameters internally defined in H2O92D routine (Johnson et al., 1992)
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H2 (AQ)                                 Source GIB500        Data type GIB
hydrogen aqueous  stefansson 2002 appendix b
      a            b            c            d            e            f
-19666.6      780.435     0.348833     -.168301E-03 0.000000     -138.360
Tmin =   25.00 C      Tmax =  460.00 C

O H E (AQ)                              Source ETHAQU95      Data type ETH
HKF species: OH-
 DfH = -54977.0 cal/mol                  S = -2.56000 cal/K/mol
  a1 = 0.125270 cal/bar/mol             a2 = 7.38000 cal/mol
  a3 = 1.84230 cal*K/bar/mol            a4 = -27821.0 cal*K/mol
  c1 = 4.15000 cal/K/mol                c2 = -103460. cal*K/mol
   w = 172460. cal/mol                   Z = -1

H CL (AQ)                               Source GIB500        Data type GIB
hydrogen chloride ion pair stefansson 2002 appendix b
      a            b            c            d            e            f
-27475.1     -540.563     -.240603     0.671611E-04 0.000000      104.818
Tmin =   25.00 C      Tmax =  460.00 C

H E-1 (AQ)                              Source ETHAQU95      Data type ETH
HKF species: H+
 DfH = 0.000000 cal/mol                  S = 0.000000 cal/K/mol
  a1 = 0.000000 cal/bar/mol             a2 = 0.000000 cal/mol
  a3 = 0.000000 cal*K/bar/mol           a4 = 0.000000 cal*K/mol
  c1 = 0.000000 cal/K/mol               c2 = 0.000000 cal*K/mol
   w = 0.000000 cal/mol                  Z = 1

NA CL (AQ)                              Source ETHAQU95      Data type ETH
HKF species: NACL
 DfH = -96120.0 cal/mol                  S = 28.0000 cal/K/mol
  a1 = 0.503630 cal/bar/mol             a2 = 473.650 cal/mol
  a3 = 3.41540 cal*K/bar/mol            a4 = -29748.0 cal*K/mol
  c1 = 10.8000 cal/K/mol                c2 = -13000.0 cal*K/mol
   w = -3800.00 cal/mol                  Z = 0

NA E-1 (AQ)                             Source ETHAQU95      Data type ETH
HKF species: NA+
 DfH = -57433.0 cal/mol                  S = 13.9600 cal/K/mol
  a1 = 0.183900 cal/bar/mol             a2 = -228.500 cal/mol
  a3 = 3.25600 cal*K/bar/mol            a4 = -27260.0 cal*K/mol
  c1 = 18.1800 cal/K/mol                c2 = -29810.0 cal*K/mol
   w = 33060.0 cal/mol                   Z = 1

Na O H (AQ)                             Source GIB500        Data type GIB
sodium hydroxide ion pair, stefansson 2002 appendix b
      a            b            c            d            e            f
-90246.4     -507.136     -.117207     0.283613E-04 0.000000      89.3935
Tmin =   25.00 C      Tmax =  460.00 C

K CL (AQ)                               Source ETHAQU95      Data type ETH
HKF species: KCL
 DfH = -97400.0 cal/mol                  S = 39.1000 cal/K/mol
  a1 = 0.723860 cal/bar/mol             a2 = 989.280 cal/mol
  a3 = 1.86160 cal*K/bar/mol            a4 = -31880.0 cal*K/mol
  c1 = -1.43400 cal/K/mol               c2 = 60310.0 cal*K/mol
   w = -3000.00 cal/mol                  Z = 0
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```
K E-1 (AQ)                                Source ETHAQU95      Data type ETH
HKF species: K+
 DfH = -60270.0 cal/mol                    S = 24.1500 cal/K/mol
  a1 = 0.355900 cal/bar/mol               a2 = -147.300 cal/mol
  a3 = 5.43500 cal*K/bar/mol              a4 = -27120.0 cal*K/mol
  c1 = 7.40000 cal/K/mol                  c2 = -17910.0 cal*K/mol
   w = 19270.0 cal/mol                     Z = 1

CL E (AQ)                                 Source ETHAQU95      Data type ETH
HKF species: CL-
 DfH = -39933.0 cal/mol                    S = 13.5600 cal/K/mol
  a1 = 0.403200 cal/bar/mol               a2 = 480.100 cal/mol
  a3 = 5.56300 cal*K/bar/mol              a4 = -28470.0 cal*K/mol
  c1 = -4.40000 cal/K/mol                 c2 = -57140.0 cal*K/mol
   w = 145600. cal/mol                     Z = -1

FeCl2 (aq)                                Source ETHAQU95      Data type ETH
HKF species: FECL2
 DfH = -78490.0 cal/mol                    S = 43.0000 cal/K/mol
  a1 = 0.571500 cal/bar/mol               a2 = 617.240 cal/mol
  a3 = 3.32580 cal*K/bar/mol              a4 = -30341.0 cal*K/mol
  c1 = 22.3084 cal/K/mol                  c2 = 26975.0 cal*K/mol
   w = -3800.00 cal/mol                    Z = 0

FeCl E-1 (aq)                             Source ETHAQU95      Data type ETH
HKF species: FECL+
 DfH = -61260.0 cal/mol                    S = -10.0600 cal/K/mol
  a1 = 0.207560 cal/bar/mol               a2 = -271.290 cal/mol
  a3 = 6.81440 cal*K/bar/mol              a4 = -26667.0 cal*K/mol
  c1 = 24.6737 cal/K/mol                  c2 = 11555.0 cal*K/mol
   w = 70030.0 cal/mol                     Z = 1

Fe E-2 (aq)                               Source ETHAQU95      Data type ETH
HKF species: FE+2
 DfH = -22050.0 cal/mol                    S = -25.3000 cal/K/mol
  a1 = -.780300E-01 cal/bar/mol           a2 = -968.670 cal/mol
  a3 = 9.55730 cal*K/bar/mol              a4 = -23786.0 cal*K/mol
  c1 = 14.9632 cal/K/mol                  c2 = -46438.0 cal*K/mol
   w = 145740. cal/mol                     Z = 2

H2S (aq)                                  Source ETHAQU95      Data type ETH
HKF species: H2S
 DfH = -9325.00 cal/mol                    S = 30.0000 cal/K/mol
  a1 = 0.650970 cal/bar/mol               a2 = 677.240 cal/mol
  a3 = 5.96460 cal*K/bar/mol              a4 = -30590.0 cal*K/mol
  c1 = 32.3000 cal/K/mol                  c2 = 47300.0 cal*K/mol
   w = -10000.0 cal/mol                    Z = 0

H S E (aq)                                Source GIB500        Data type GIB
bisulfide ion stefansson 2002 appendix b
      a            b            c            d            e            f
 121697.     -4831.91     -2.01172     0.803862E-03 0.000000      870.949
Tmin =   25.00 C      Tmax =  460.00 C
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```
Na H S (aq)                              Source GIB500        Data type GIB
sodium bisulfide ion pair stefansson 2002 appendix b
      a            b           c            d            e            f
 7197.78     -2387.05     -.886099     0.317759E-03 0.000000      422.047
Tmin =   25.00 C      Tmax =  460.00 C

S O2 (aq)                               Source ETHAQU95      Data type ETH
 HKF species: SO2
  DfH = -77194.0 cal/mol                  S = 38.7000 cal/K/mol
   a1 = 0.695020 cal/bar/mol             a2 = 918.900 cal/mol
   a3 = 2.13830 cal*K/bar/mol            a4 = -31589.0 cal*K/mol
   c1 = 31.2101 cal/K/mol                c2 = 64578.0 cal*K/mol
    w = -24610.0 cal/mol                  Z = 0

 H S O3 E (aq)                          Source ETHAQU95      Data type ETH
 HKF species: HSO3-
  DfH = -149670. cal/mol                  S = 33.4000 cal/K/mol
   a1 = 0.670140 cal/bar/mol             a2 = 858.160 cal/mol
   a3 = 2.37710 cal*K/bar/mol            a4 = -31338.0 cal*K/mol
   c1 = 15.6949 cal/K/mol                c2 = -33198.0 cal*K/mol
    w = 112330. cal/mol                   Z = -1

 S O3 e2 (aq)                           Source ETHAQU95      Data type ETH
 HKF species: SO3-2
  DfH = -151900. cal/mol                  S = -7.00000 cal/K/mol
   a1 = 0.365370 cal/bar/mol             a2 = 31.9100 cal/mol
   a3 = 7.38530 cal*K/bar/mol            a4 = -27922.0 cal*K/mol
   c1 = -7.83680 cal/K/mol               c2 = -185362. cal*K/mol
    w = 332100. cal/mol                   Z = -2

 H S O4 E (aq)                          Source ETHAQU95      Data type ETH
 HKF species: HSO4-
  DfH = -212500. cal/mol                  S = 30.0000 cal/K/mol
   a1 = 0.697880 cal/bar/mol             a2 = 925.900 cal/mol
   a3 = 2.11080 cal*K/bar/mol            a4 = -31618.0 cal*K/mol
   c1 = 20.0961 cal/K/mol                c2 = -19550.0 cal*K/mol
    w = 117480. cal/mol                   Z = -1

 S O4 e2 (aq)                           Source ETHAQU95      Data type ETH
 HKF species: SO4-2
  DfH = -217400. cal/mol                  S = 4.50000 cal/K/mol
   a1 = 0.830140 cal/bar/mol             a2 = -198.460 cal/mol
   a3 = -6.21220 cal*K/bar/mol           a4 = -26970.0 cal*K/mol
   c1 = 1.64000 cal/K/mol                c2 = -179980. cal*K/mol
    w = 314630. cal/mol                   Z = -2

 Na S O4 E (aq)                         Source ETHCH03       Data type ETH
 HKF species: NASO4- ESTIMATED FROM KSO4-KCL+NASO4 OF ETHAQU95
  DfH = -275699. cal/mol                  S = 23.9006 cal/K/mol
   a1 = 0.387531 cal/bar/mol             a2 = 190.069 cal/mol
   a3 = 4.53290 cal*K/bar/mol            a4 = -28574.1 cal*K/mol
   c1 = 22.0842 cal/K/mol                c2 = -126062. cal*K/mol
    w = 109160. cal/mol                   Z = -1
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K S O4 E (aq)                          Source ETHAQU95      Data type ETH
HKF species: KSO4-
 DfH = -276980. cal/mol                 S = 35.0000 cal/K/mol
  a1 = 0.607760 cal/bar/mol            a2 = 705.700 cal/mol
  a3 = 2.97910 cal*K/bar/mol           a4 = -30706.0 cal*K/mol
  c1 = 9.85020 cal/K/mol               c2 = -52752.0 cal*K/mol
   w = 109960. cal/mol                  Z = -1

Si O2 (aq)                             Source ETHAQU95      Data type ETH
HKF species: SIO2
 DfH = -209775. cal/mol                 S = 18.0000 cal/K/mol
  a1 = 0.190000 cal/bar/mol            a2 = 170.000 cal/mol
  a3 = 20.0000 cal*K/bar/mol           a4 = -27000.0 cal*K/mol
  c1 = 29.1000 cal/K/mol               c2 = -512000. cal*K/mol
   w = 12910.0 cal/mol                  Z = 0

Au H S(aq)                             Source GIB500        Data type GIB
gold bisulfide complex  stefansson 2002
      a            b            c            d            e            f
-257851.      10250.1      4.04321     -.141701E-02 0.000000     -1832.13
Tmin =   25.00 C      Tmax =  460.00 C

AuH2S2E(aq)                            Source GIB500        Data type GIB
gold disulfide complex ion stefansson 2002
      a            b            c            d            e            f
-69036.9      3451.78      1.66046     -.586167E-03 0.000000     -641.044
Tmin =   25.00 C      Tmax =  460.00 C

Au Cl2 E (aq)                          Source GIB500        Data type GIB
gold dichloride ion stefansson 2002
      a            b            c            d            e            f
 328065.     -13866.7     -5.41498     0.199543E-02 0.000000      2471.87
Tmin =   25.00 C      Tmax =  460.00 C

Au O H (aq)                            Source GIB500        Data type GIB
gold hydroxyl complex  stefansson 2002
      a            b            c            d            e            f
-3384.50     -459.472     -.432922E-01 0.377723E-04 0.000000      68.7539
Tmin =   25.00 C      Tmax =  460.00 C

K AL SI3 O8                            Source ETHMIN95      Data type ETH
SUPCRT mineral: K-FELDSPAR
 DfH = -950944. cal/mol  S = 51.1300 cal/K/mol  V = 108.870 cc/mol
  Cp = 76.6170 + (0.431100E-02*T) + (-.299450E+07/T/T)
Tmax = 1126.85 C                      DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                dPdT = 0.000000 bar/K

NAALSI3 O8                             Source ETHMIN95      Data type ETH
SUPCRT mineral: ALBITE,LOW
 DfH = -942342. cal/mol  S = 49.5100 cal/K/mol  V = 100.070 cc/mol
  Cp = 61.7000 + (0.139000E-01*T) + (-.150100E+07/T/T)
Tmax = 1126.85 C                      DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                dPdT = 0.000000 bar/K
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K AL3 SI3 O12 H2                        Source ETHMIN95      Data type ETH
SUPCRT mineral: MUSCOVITE
 DfH = -.143151E+07 cal/mol  S = 68.8000 cal/K/mol  V = 140.810 cc/mol
  Cp = 74.8650 + (0.662030E-01*T) + (-.148120E+07/T/T)
Tmax = 224.25 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K
  Cp = 116.057 + (0.109920E-01*T) + (-.487830E+07/T/T)
Tmax = 726.85 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

Al2 Si2 O9H4                            Source ETHMIN95      Data type ETH
SUPCRT mineral: KAOLINITE
 DfH = -985307. cal/mol  S = 48.0200 cal/K/mol  V = 99.5200 cc/mol
  Cp = 59.4610 + (0.485750E-01*T) + (-.132930E+07/T/T)
Tmax = 450.00 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

Al2 Si4  O12 H2                         Source ETHMIN95      Data type ETH
SUPCRT mineral: PYROPHYLLITE
 DfH = -.134839E+07 cal/mol  S = 57.2000 cal/K/mol  V = 127.820 cc/mol
  Cp = 75.0000 + (0.480060E-01*T) + (-.169900E+07/T/T)
Tmax = 726.85 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

Al2Si O5                                Source ETHMIN95      Data type ETH
SUPCRT mineral: ANDALUSITE
 DfH = -618815. cal/mol  S = 22.2000 cal/K/mol  V = 51.5300 cc/mol
  Cp = 41.3108 + (0.629256E-02*T) + (-.123921E+07/T/T)
Tmax = 769.85 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

SI O2                                   Source ETHMIN95      Data type ETH
SUPCRT mineral: QUARTZ
 DfH = -217660. cal/mol  S = 9.88000 cal/K/mol  V = 22.6880 cc/mol
  Cp = 11.2200 + (0.820000E-02*T) + (-270000./T/T)
Tmax = 574.85 C                         DtrH = 290.000 cal/mol
DtrV = 0.372000 cc/mol                  dPdT = 38.5000 bar/K
  Cp = 14.4100 + (0.194000E-02*T) + (0.000000/T/T)
Tmax = 1726.85 C                        DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

Al O2 H                                 Source ETHMIN95      Data type ETH
SUPCRT mineral: BOEHMITE
 DfH = -238240. cal/mol  S = 8.89000 cal/K/mol  V = 19.5350 cc/mol
  Cp = 12.9020 + (0.124210E-01*T) + (-322800./T/T)
Tmax = 626.85 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

K Al3 S2 O14  H6                        Source CPDCH03       Data type CPD
alunite stoffregen et al. 2000 MSA Reviews
DfH = -.123561E+07 cal/mol  S = 78.3939 cal/K/mol
Cp = 153.449 + (0.000000*T) + (0.000000*T*T) + (0.549498E+07/T/T)
Tmax = 450.000 C      DtrH = 0.000000 cal/mol
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FeS2                                    Source ETHMIN95      Data type ETH
SUPCRT mineral: PYRITE
 DfH = -41000.0 cal/mol  S = 12.6500 cal/K/mol  V = 23.9400 cc/mol
  Cp = 17.8800 + (0.132000E-02*T) + (-305000./T/T)
Tmax = 726.85 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

FeS                                     Source ETHMIN95      Data type ETH
SUPCRT mineral: PYRRHOTITE
 DfH = -24000.0 cal/mol  S = 14.4100 cal/K/mol  V = 18.2000 cc/mol
  Cp = 5.19000 + (0.264000E-01*T) + (0.000000/T/T)
Tmax = 137.85 C                         DtrH = 570.000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K
  Cp = 17.4000 + (0.000000*T) + (0.000000/T/T)
Tmax = 324.85 C                         DtrH = 120.000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K
  Cp = 12.2000 + (0.238000E-02*T) + (0.000000/T/T)
Tmax = 1194.85 C                        DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

Fe3 O4                                  Source ETHMIN95      Data type ETH
SUPCRT mineral: MAGNETITE
 DfH = -267250. cal/mol  S = 34.8300 cal/K/mol  V = 44.5240 cc/mol
  Cp = 21.8800 + (0.482000E-01*T) + (0.000000/T/T)
Tmax = 626.85 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K
  Cp = 48.0000 + (0.000000*T) + (0.000000/T/T)
Tmax = 1526.85 C                        DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

Fe2 O3                                  Source ETHMIN95      Data type ETH
SUPCRT mineral: HEMATITE
 DfH = -197720. cal/mol  S = 20.9400 cal/K/mol  V = 30.2740 cc/mol
  Cp = 23.4900 + (0.186000E-01*T) + (-355000./T/T)
Tmax = 676.85 C                         DtrH = 160.000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K
  Cp = 36.0000 + (0.000000*T) + (0.000000/T/T)
Tmax = 776.85 C                         DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K
  Cp = 31.7100 + (0.176000E-02*T) + (0.000000/T/T)
Tmax = 1526.85 C                        DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K

Au                                      Source ETHMIN95      Data type ETH
SUPCRT mineral: GOLD,NATIVE
 DfH = 0.000000 cal/mol  S = 11.3300 cal/K/mol  V = 10.2150 cc/mol
  Cp = 5.66000 + (0.124000E-02*T) + (0.000000/T/T)
Tmax = 1062.85 C                        DtrH = 0.000000 cal/mol
DtrV = 0.000000 cc/mol                  dPdT = 0.000000 bar/K
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S                                        Source CPDMRL        Data type CPD
sulfur alpha beta liquid
DfH = 0.000000 cal/mol  S = 7.60000 cal/K/mol
Cp = 3.53000 + (0.575000E-02*T) + (0.000000*T*T) + (17400.0/T/T)
Tmax = 95.3900 C      DtrH = 96.0000 cal/mol
Cp = 3.56000 + (0.696000E-02*T) + (0.000000*T*T) + (0.000000/T/T)
Tmax = 115.210 C      DtrH = 410.500 cal/mol
Cp = 24858.9 + (-81.7675*T) + (0.756363E-01*T*T) + (-.679311E+09/T/T)
Tmax = 159.100 C      DtrH = 0.000000 cal/mol
Cp = -100.456 + (0.237724*T) + (-.147320E-03*T*T) + (0.686637E+07/T/T)
Tmax = 444.600 C      DtrH = 0.000000 cal/mol
Cp = 7.69400 + (0.000000*T) + (0.000000*T*T) + (0.000000/T/T)
Tmax = 926.850 C      DtrH = 0.000000 cal/mol
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