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 subsystem (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.

Computation shown in this paper were restricted to a segment of isobaric cooling at 500 bar 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 (2001) for Bajo de la Alumbrera and unpublished data for the Bingham porphyry-Cu-Au deposit indicate that little or no gold and sulfide precipitation occurs above 450°C, in agreement with published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 / 500 bar, 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 Stefánsson (2003).
### 2. Species list and data sources

<table>
<thead>
<tr>
<th>Species</th>
<th>Data Source</th>
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<tr>
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<td>H(_2)(g)</td>
<td>Turnbull and Wadsley (1986) CPDMRL</td>
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Species list and data sources (Continued)

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<td>and</td>
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<td>Turnbull and Wadsley (1986)</td>
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<tr>
<td>S</td>
<td>S</td>
<td>Turnbull and Wadsley (1986)</td>
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</table>

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


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

\[
D_f G (500 \text{ bar}) = a + bT + cT^2 + dT^3 + e/T + fT\ln(T) \text{ in cal/mol, where } T \text{ is the temperature in K}
\]

H2 (G)  Source CPDMRL  Data type CPD
hydrogen diatomic gas
\[
D_f H = 0.000000 \text{ cal/mol} \quad S = 31.2070 \text{ cal/K/mol}
\]
\[
C_p = 7.18062 + (-0.592740E-03*T) + (0.641294E-06*T*T) + (-14285.2/T/T)
\]
\[
T_{max} = 1226.85 \text{ C} \quad D_{tr} H = 0.000000 \text{ cal/mol}
\]

S2 (g)  Source CPDMRL  Data type CPD
sulfur gas diatomic
\[
D_f H = 30840.0 \text{ cal/mol} \quad S = 54.5100 \text{ cal/K/mol}
\]
\[
C_p = 7.55235 + (0.275658E-02*T) + (-0.149540E-05*T*T) + (-42965.1/T/T)
\]
\[
T_{max} = 526.850 \text{ C} \quad D_{tr} H = 0.000000 \text{ cal/mol}
\]

H2O (G)  Source CPDMRL  Data type CPD
hydrogen oxide gas water steam
\[
D_f H = -57798.0 \text{ cal/mol} \quad S = 45.1060 \text{ cal/K/mol}
\]
\[
C_p = 6.92691 + (-0.264398E-02*T) + (0.255648E-06*T*T) + (25572.3/T/T)
\]
\[
T_{max} = 726.850 \text{ C} \quad D_{tr} H = 0.000000 \text{ cal/mol}
\]

H2S (g)  Source CPDMRL  Data type CPD
hydrogen sulfide gas
\[
D_f H = -4880.00 \text{ cal/mol} \quad S = 49.1510 \text{ cal/K/mol}
\]
\[
C_p = 7.81000 + (0.296000E-02*T) + (0.000000*T*T) + (-46000.0/T/T)
\]
\[
T_{max} = 2026.85 \text{ C} \quad D_{tr} H = 0.000000 \text{ cal/mol}
\]

N2 (g)  Source CPDMRL  Data type CPD
nitrogen diatomic gas
\[
D_f H = 0.000000 \text{ cal/mol} \quad S = 45.7700 \text{ cal/K/mol}
\]
\[
C_p = 6.51773 + (0.560719E-03*T) + (0.811435E-06*T*T) + (18257.7/T/T)
\]
\[
T_{max} = 526.850 \text{ C} \quad D_{tr} H = 0.000000 \text{ cal/mol}
\]

H2 O (AQ)  Source ETHAQU95  Data type ETH
Parameters internally defined in H2O92D routine (Johnson et al., 1992)
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  -0.168301E-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  
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  
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  
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  
Tmin =  25.00 C  
Tmax =  460.00 C

NA CL (AQ)  
Source ETHAQU95  
Data type ETH  
HKF species: NACL  
DfH = -96120.0 cal/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  
Tmin =  25.00 C  
Tmax =  460.00 C

NA E-1 (AQ)  
Source ETHAQU95  
Data type ETH  
HKF species: NA+  
DfH = -57433.0 cal/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  
Tmin =  25.00 C  
Tmax =  460.00 C

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  
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  
Tmin =  25.00 C  
Tmax =  460.00 C

K E-1 (AQ)  
Source ETHAQU95  
Data type ETH  
HKF species: K+  
DfH = 0.000000 cal/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  
Tmin =  25.00 C  
Tmax =  460.00 C
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
cl = 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
cl = -4.40000 cal/K/mol    c2 = -57140.0 cal*K/mol
w = 145600.0 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
cl = 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
cl = 24.6737 cal/K/mol     c2 = 11555.0 cal*K/mol
w = 70030.00 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 = -7.80300E-01 cal/bar/mol a2 = -968.670 cal/mol
a3 = 9.55730 cal*K/bar/mol  a4 = -23786.0 cal*K/mol
cl = 14.9632 cal/K/mol     c2 = -46438.0 cal*K/mol
w = 145740.0 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
cl = 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
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Na H S (aq)                            Source GIB500        Data type GIB
sodium bisulfide ion pair stefansson 2002 appendix b

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<thead>
<tr>
<th>a</th>
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<th>c</th>
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Tmin = 25.00 C  Tmax = 460.00 C

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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 = 422.047

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 = -26970.0 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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<td>( a_1 = 0.607760 \text{ cal/bar/mol} ) &amp; ( a_2 = 705.700 \text{ cal/mol} )</td>
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<td>( a_3 = 2.97910 \text{ cal/K/bar/mol} ) &amp; ( a_4 = -30706.0 \text{ cal/K/mol} )</td>
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<td>( c_1 = 9.85020 \text{ cal/K/mol} ) &amp; ( c_2 = -52752.0 \text{ cal/K/mol} )</td>
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<td>( w = 109960. \text{ cal/mol} ) &amp; ( Z = -1 )</td>
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<td>( S = 18.0000 \text{ cal/K/mol} )</td>
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<tr>
<td>( a_1 = 0.190000 \text{ cal/bar/mol} ) &amp; ( a_2 = 170.000 \text{ cal/mol} )</td>
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</tr>
<tr>
<td>( a_3 = 20.0000 \text{ cal/K/bar/mol} ) &amp; ( a_4 = -27000.0 \text{ cal/K/mol} )</td>
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<td></td>
</tr>
<tr>
<td>( c_1 = 29.1000 \text{ cal/K/mol} ) &amp; ( c_2 = -512000. \text{ cal/K/mol} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( w = 12910.0 \text{ cal/mol} ) &amp; ( Z = 0 )</td>
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<td></td>
</tr>
<tr>
<td>AuH2S2E(aq)</td>
<td>GIB500</td>
<td>GIB</td>
</tr>
<tr>
<td>gold bisulfide complex stefansson 2002</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| \begin{tabular}{cccccc}
| a     | b     | c     | d     | e     | f     |
| \(-257851.0\) | \(10250.1\) | \(4.04321\) | \(-.141701E-02\) | \(0.000000\) | \(-1832.13\) |
\end{tabular} &             |           |
| Tmin = 25.00 C & Tmax = 460.00 C |
| AuCl2E(aq)                     | GIB500      | GIB       |
| gold dichloride ion stefansson 2002 |             |           |
| \begin{tabular}{cccccc}
| a     | b     | c     | d     | e     | f     |
| \(-69036.9\) | \(3451.78\) | \(1.66046\) | \(-.586167E-03\) | \(0.000000\) | \(-641.044\) |
\end{tabular} &             |           |
| Tmin = 25.00 C & Tmax = 460.00 C |
| AuOH(aq)                       | GIB500      | GIB       |
| gold hydroxyl complex stefansson 2002 |             |           |
| \begin{tabular}{cccccc}
| a     | b     | c     | d     | e     | f     |
| \(-3384.50\) | \(-459.472\) | \(-.432922E-01\) | \(0.377723E-04\) | \(0.000000\) | \(68.7539\) |
\end{tabular} &             |           |
| Tmin = 25.00 C & Tmax = 460.00 C |
| KALSI3O8                       | ETHMIN95    | ETH       |
| SUPCRT mineral: K-FELDSPAR     |             |           |
| \( \Delta f H \) = -950944. cal/mol | \( S = 51.1300 \text{ cal/K/mol} \) \( V = 108.870 \text{ cc/mol} \) |
| \( C_p = 76.6170 + (0.431100E-02*T) + (-.299450E+07/T/T) \) & \( T_{max} = 1126.85 \text{ C} \) |
| \( D_{trH} = 0.000000 \text{ cal/mol} \) & \( D_{trV} = 0.000000 \text{ bar/K} \) |
| NAALSI3O8                      | ETHMIN95    | ETH       |
| SUPCRT mineral: ALBITE,LOW     |             |           |
| \( \Delta f H \) = -942342. cal/mol | \( S = 49.5100 \text{ cal/K/mol} \) \( V = 100.070 \text{ cc/mol} \) |
| \( C_p = 61.7000 + (0.139000E-01*T) + (-.150100E+07/T/T) \) & \( T_{max} = 1126.85 \text{ C} \) |
| \( D_{trH} = 0.000000 \text{ cal/mol} \) & \( D_{trV} = 0.000000 \text{ bar/K} \) |
K Al$_3$ Si$_3$ O$_{12}$ H$_2$  

**SUPCRT mineral: MUSCOVITE**

- $D_{fH} = -1.43151E+07$ cal/mol  
- $S = 68.8000$ cal/K/mol  
- $V = 140.810$ cc/mol

**Data** ETHMIN95  

- $C_p = 74.8650 + (0.662030E-01*T) + (-.148120E+07/T/T)$
- $T_{max} = 224.25$ C  
- $D_{trH} = 0.00000$ cal/mol  
- $D_{trV} = 0.00000$ cc/mol  
- $d_{PdT} = 0.00000$ bar/K

Al$_2$ Si$_2$ O$_9$ H$_4$

**SUPCRT mineral: KAOLINITE**

- $D_{fH} = -985307.$ cal/mol  
- $S = 48.0200$ cal/K/mol  
- $V = 99.5200$ cc/mol

**Data** ETHMIN95  

- $C_p = 59.4610 + (0.485750E-01*T) + (-.132930E+07/T/T)$
- $T_{max} = 450.00$ C  
- $D_{trH} = 0.00000$ cal/mol  
- $D_{trV} = 0.00000$ cc/mol  
- $d_{PdT} = 0.00000$ bar/K

Al$_2$ Si$_4$ O$_{12}$ H$_2$

**SUPCRT mineral: PYROPHYLLITE**

- $D_{fH} = -1.34839E+07$ cal/mol  
- $S = 57.2000$ cal/K/mol  
- $V = 127.820$ cc/mol

**Data** ETHMIN95  

- $C_p = 75.0000 + (0.480060E-01*T) + (-.169900E+07/T/T)$
- $T_{max} = 726.85$ C  
- $D_{trH} = 0.00000$ cal/mol  
- $D_{trV} = 0.00000$ cc/mol  
- $d_{PdT} = 0.00000$ bar/K

Al$_2$Si O$_5$

**SUPCRT mineral: ANDALUSITE**

- $D_{fH} = -618815.$ cal/mol  
- $S = 22.2000$ cal/K/mol  
- $V = 51.5300$ cc/mol

**Data** ETHMIN95  

- $C_p = 41.3108 + (0.629256E-02*T) + (-.123921E+07/T/T)$
- $T_{max} = 769.85$ C  
- $D_{trH} = 0.00000$ cal/mol  
- $D_{trV} = 0.00000$ cc/mol  
- $d_{PdT} = 0.00000$ bar/K

Si O$_2$

**SUPCRT mineral: QUARTZ**

- $D_{fH} = -217660.$ cal/mol  
- $S = 9.88000$ cal/K/mol  
- $V = 22.6880$ cc/mol

**Data** ETHMIN95  

- $C_p = 11.2200 + (0.820000E-02*T) + (-270000./T/T)$
- $T_{max} = 769.85$ C  
- $D_{trH} = 0.00000$ cal/mol  
- $D_{trV} = 0.00000$ cc/mol  
- $d_{PdT} = 0.00000$ bar/K

Al O$_2$ H

**SUPCRT mineral: BOEHMITE**

- $D_{fH} = -238240.$ cal/mol  
- $S = 8.89000$ cal/K/mol  
- $V = 19.5350$ cc/mol

**Data** ETHMIN95  

- $C_p = 12.9020 + (0.124210E-01*T) + (-322800./T/T)$
- $T_{max} = 626.85$ C  
- $D_{trH} = 0.00000$ cal/mol  
- $D_{trV} = 0.00000$ cc/mol  
- $d_{PdT} = 0.00000$ bar/K

K Al$_3$ S$_2$ O$_{14}$ H$_6$

**SUPCRT mineral: alunite**

- $D_{fH} = -1.23561E+07$ cal/mol  
- $S = 78.3939$ cal/K/mol  
- $C_p = 153.449 + (0.000000*T) + (0.000000*T*T) + (0.549498E+07/T/T)$
- $T_{max} = 450.000$ C  
- $D_{trH} = 0.00000$ cal/mol
<table>
<thead>
<tr>
<th>Mineral</th>
<th>Source</th>
<th>Data type</th>
</tr>
</thead>
<tbody>
<tr>
<td>FeS2</td>
<td>ETHMIN95</td>
<td>ETH</td>
</tr>
<tr>
<td>SUPCRT mineral: PYRITE</td>
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<tr>
<td>$\Delta_f H = -41000.0$ cal/mol</td>
<td>$S = 12.6500$ cal/K/mol</td>
<td>$V = 23.9400$ cc/mol</td>
</tr>
<tr>
<td>$C_p = 17.8800 + (0.132000E-02 \times T) + (-305000 ./T/T)$</td>
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</tr>
<tr>
<td>$T_{max} = 726.85 \degree C$</td>
<td>$\Delta r H = 0.000000$ cal/mol</td>
<td>$dPdT = 0.000000$ bar/K</td>
</tr>
<tr>
<td>$\Delta r V = 0.000000$ cc/mol</td>
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</tr>
<tr>
<td>FeS</td>
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<td>ETH</td>
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<tr>
<td>SUPCRT mineral: PYRRHOTITE</td>
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<td>$\Delta_f H = -24000.0$ cal/mol</td>
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<td>$V = 18.2000$ cc/mol</td>
</tr>
<tr>
<td>$C_p = 5.19000 + (0.264000E-01 \times T) + (0.000000/T/T)$</td>
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<tr>
<td>$T_{max} = 137.85 \degree C$</td>
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<td>$dPdT = 0.000000$ bar/K</td>
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<td>$\Delta r V = 0.000000$ cc/mol</td>
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<tr>
<td>$C_p = 17.4000 + (0.238000E-02 \times T) + (0.000000/T/T)$</td>
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<td>$T_{max} = 324.85 \degree C$</td>
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<td>$\Delta r V = 0.000000$ cc/mol</td>
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<tr>
<td>Fe3 O4</td>
<td>ETHMIN95</td>
<td>ETH</td>
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<tr>
<td>SUPCRT mineral: MAGNETITE</td>
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<td>$\Delta_f H = -267250.$ cal/mol</td>
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<tr>
<td>$C_p = 21.8800 + (0.482000E-01 \times T) + (0.000000/T/T)$</td>
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</tr>
<tr>
<td>$T_{max} = 626.85 \degree C$</td>
<td>$\Delta r H = 0.000000$ cal/mol</td>
<td>$dPdT = 0.000000$ bar/K</td>
</tr>
<tr>
<td>$\Delta r V = 0.000000$ cc/mol</td>
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</tr>
<tr>
<td>$C_p = 48.0000 + (0.000000 \times T) + (0.000000/T/T)$</td>
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<tr>
<td>$T_{max} = 1526.85 \degree C$</td>
<td>$\Delta r H = 160.000$ cal/mol</td>
<td>$dPdT = 0.000000$ bar/K</td>
</tr>
<tr>
<td>$\Delta r V = 0.000000$ cc/mol</td>
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</tr>
<tr>
<td>Fe2 O3</td>
<td>ETHMIN95</td>
<td>ETH</td>
</tr>
<tr>
<td>SUPCRT mineral: HEMATITE</td>
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<tr>
<td>$\Delta_f H = -197720.$ cal/mol</td>
<td>$S = 20.9400$ cal/K/mol</td>
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</tr>
<tr>
<td>$\Delta r V = 0.000000$ cc/mol</td>
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</tr>
<tr>
<td>$C_p = 31.7100 + (0.176000E-02 \times T) + (0.000000/T/T)$</td>
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<td></td>
</tr>
<tr>
<td>$T_{max} = 1526.85 \degree C$</td>
<td>$\Delta r H = 0.000000$ cal/mol</td>
<td>$dPdT = 0.000000$ bar/K</td>
</tr>
<tr>
<td>$\Delta r V = 0.000000$ cc/mol</td>
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</tr>
<tr>
<td>Au</td>
<td>ETHMIN95</td>
<td>ETH</td>
</tr>
<tr>
<td>SUPCRT mineral: GOLD,NATIVE</td>
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</tr>
<tr>
<td>$\Delta_f H = 0.000000$ cal/mol</td>
<td>$S = 11.3300$ cal/K/mol</td>
<td>$V = 10.2150$ cc/mol</td>
</tr>
<tr>
<td>$C_p = 5.66000 + (0.124000E-02 \times T) + (0.000000/T/T)$</td>
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</tr>
<tr>
<td>$T_{max} = 1062.85 \degree C$</td>
<td>$\Delta r H = 0.000000$ cal/mol</td>
<td>$dPdT = 0.000000$ bar/K</td>
</tr>
<tr>
<td>$\Delta r V = 0.000000$ cc/mol</td>
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</tr>
</tbody>
</table>
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