

Thermodynamic Properties  
of Minerals and Related  
Substances at 298.15 K and  
1 Bar ( $10^5$  Pascals) Pressure  
and at Higher Temperatures

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U.S. GEOLOGICAL SURVEY BULLETIN 1452





# Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar ( $10^5$ Pascals) Pressure and at Higher Temperatures

By RICHARD A. ROBIE, BRUCE S. HEMINGWAY, and JAMES R. FISHER

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*A summary of the thermodynamic data for minerals at 298.15 K together with calculated values for the functions  $C_{P,T}^{\circ}$ ,  $\Delta H_{f,T}^{\circ}$ ,  $\Delta G_{f,T}^{\circ}$ ,  $S_T^{\circ}$ ,  $(H_T^{\circ} - H_{298}^{\circ})/T$ , and  $(G_T^{\circ} - H_{298}^{\circ})/T$  at temperatures up to 1,800 K*



Reprinted with corrections 1979

DEPARTMENT OF THE INTERIOR

WILLIAM P. CLARK, *Secretary*

U.S. GEOLOGICAL SURVEY

Dallas L. Peck, *Director*

First printing 1978  
Second printing 1979  
Third printing 1984



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# THERMODYNAMIC PROPERTIES OF MINERALS AND RELATED SUBSTANCES AT 298.15 K AND 1 BAR ( $10^5$ PASCALS) PRESSURE AND AT HIGHER TEMPERATURES

By RICHARD A. ROBIE, BRUCE S. HEMINGWAY, and JAMES R. FISHER

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## ABSTRACT

Selected values for the entropy ( $S^\circ$ ), molar volume ( $v^\circ$ ), and for the enthalpy and Gibbs free energy of formation ( $\Delta H_f^\circ$  and  $\Delta G_f^\circ$ ) are given for the elements, 133 oxides, and 212 other minerals and related substances at 298.15 K. For those materials for which high-temperature heat-capacity or heat-content data are also available ( $(H_T^\circ - H_{298}^\circ)/T$ ,  $S_T^\circ$ ,  $(G_T^\circ - H_{298}^\circ)/T$ ,  $C_p^\circ$ ,  $\Delta H_{f,T}^\circ$ ,  $\Delta G_{f,T}^\circ$  and  $\log K_{f,T}$  are tabulated at 100 K intervals for temperatures up to 1,800 K. For substances that have solid-state phase changes or whose melting or boiling point is less than 1,800 K, we have also tabulated the properties listed above at the temperature of the phase change so that the enthalpy or entropy changes associated with the transformation form an integral part of the high-temperature tables.

## INTRODUCTION

The purpose of these tables of thermodynamic properties is to present a critical summary of the available thermodynamic data for minerals and related substances in a convenient form for the use of earth scientists. To make the tables as useful as possible, we have tried (1) to include enough auxiliary data so that a single set of tables would suffice for most calculations, (2) to insure internal consistency, and (3) to provide the means for rapid revision and expansion as new data become available.

This compilation is divided into two sections. In the first section, we give values for the entropy ( $S_{298}^\circ$ ), molar volume ( $v_{298}^\circ$ ), the enthalpy of formation ( $\Delta H_{f,298}^\circ$ ) and Gibbs free energy of formation ( $\Delta G_{f,298}^\circ$ ), and the logarithm of the equilibrium constant of formation ( $\log K_{f,298}$ ) for the reference elements, minerals, several oxides, and other substances of geological interest, where the subscript 298 implies 298.15 K. The tables in the second section contain values for the thermodynamic properties at 100 K intervals for temperatures up to 1,800 K. The data are arranged in order of their conventional mineralogical groups. Within each group (for example, the oxides), the listing is by alphabetical order of the chemical symbol of the principal cation.

The data have been taken from recent critical evaluations or have been evaluated by the present authors, and uncertainties have been assigned to the 298.15 K properties. The sources of data are indicated numerically

in the tables and listed in complete form following the tables. These tables entirely supersede those of an earlier report on the same subject matter by Robie and Waldbaum (1968).

The true differential heat capacity,  $C_p^\circ$ , is rarely measured at temperatures above 400 K because of the ease with which the heat content,  $H_T^\circ - H_{298}^\circ$ , may be determined. From the heat-content measurements, one may derive approximate values for  $C_p^\circ$  at high temperatures by differentiation of the  $H_T^\circ - H_{298}^\circ$  versus temperature curve. Because many users find it more convenient to use analytical expressions for heat capacities rather than tabulated values, we have also provided equations for the heat capacities at high temperatures.

In order to derive values of  $C_p^\circ$  from the experimental heat-content measurements, the measured values of  $H_T^\circ - H_{298}^\circ$  were fitted to polynomials having six or fewer terms, and constrained so that at 298.15 K,  $H_T^\circ - H_{298}^\circ$  was identically equal to 0 and that the first derivative of the fitted equation at 298.15 K had to equal the value of the heat capacity obtained by low-temperature calorimetry. This procedure forces the values of  $C_p^\circ$  derived from the *heat-content* measurements to join smoothly with the more accurate directly measured values of  $C_p^\circ$  determined by low-temperature calorimetry.

The least-squares fitting was done by computer, using either the program HINC written by D. W. Osborne of Argonne National Laboratory (D. W. Osborne, written com., 1975) or PHAS20 (Haas and Fisher, 1976). The equation used to fit the heat-content data was that suggested by Haas and Fisher (1976).

$$H_T^\circ - H_{298}^\circ = A + BT + CT^2 + D/T + ET^{1/2} + FT^3$$

The first four terms of this equation are those used by Kelley (1960). For most phases, only four or five terms have been used. In fitting the data, we have followed a general rule that the number of experimental points should be approximately three times the number of constants used in the equation. The tabulated values of the heat capacity,  $C_p^\circ$ , at temperatures above 400 K were obtained by differentiation of the heat-content equation. The derived  $C_p^\circ$  equation, and its range of validity, is listed at the bottom of each high-temperature table.

Thermodynamic properties of gases at high pressures have not been included in these tables. High pressure-high temperature functions of the most geologically important gases,  $H_2O$  and  $CO_2$ , have been given by Bain (1964), Hilsenrath and others (1955), Robie (1966), and Burnham and others (1969).

## PHYSICAL CONSTANTS AND ATOMIC WEIGHTS

The symbols and constants used in these tables are listed in table 1. The units adopted for reporting the thermodynamic properties are those of the International System of Units (SI) (Page and Vigoureaux, 1972).

TABLE 1.—*Symbols, constants, and conversion factors*

T	Temperature in kelvins.
K	Kelvin, the unit of temperature. It is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water.
J	Joule, the unit of energy (or work). One joule = 1/4.1840 thermochemical calories or 10 cm <sup>3</sup> ·bar.
mol	Amount of substance of a system that contains as many elementary entities as there are atoms in 0.012 kilograms of carbon 12. It is identical with the gfw (gram formula weight).
P	Pressure in bars. One bar = 10 <sup>5</sup> pascals or 0.1 MPa. The standard atmosphere is equal to 101325 pascals. The kilogram·cm <sup>-2</sup> is equal to 98065.5 pascals.
°	Superscript indicates that the substance is in its standard state, 1 bar (10 <sup>5</sup> pascals) for a condensed phase.
H <sub>T</sub> <sup>°</sup> - H <sub>298</sub> <sup>°</sup>	Enthalpy at temperature T relative to 298.15 K in J·mol <sup>-1</sup> , also called the heat content.
(H <sub>T</sub> <sup>°</sup> - H <sub>298</sub> <sup>°</sup> )/T	Enthalpy function in J·mol <sup>-1</sup> ·K <sup>-1</sup> .
S <sub>T</sub> <sup>°</sup>	Entropy at temperature T, in J·mol <sup>-1</sup> ·K <sup>-1</sup> .
(G <sub>T</sub> <sup>°</sup> - H <sub>298</sub> <sup>°</sup> )/T	Gibbs energy function in J·mol <sup>-1</sup> ·K <sup>-1</sup> .
C <sub>P</sub> <sup>°</sup>	Heat capacity at constant pressure in J·mol <sup>-1</sup> ·K <sup>-1</sup> .
v <sub>298</sub> <sup>°</sup>	Volume of 1 mol of a substance at 1 bar pressure and at 298.15 K, in cm <sup>3</sup> , or J·bar <sup>-1</sup> .
ΔH <sub>m</sub> <sup>°</sup>	Enthalpy of melting at 1 bar pressure in J·mol <sup>-1</sup> .
ΔH <sub>b</sub> <sup>°</sup>	Enthalpy of vaporization to the ideal gas at 1 bar pressure at the normal boiling point in J·mol <sup>-1</sup> .
ΔH <sub>f</sub> <sup>°</sup>	Enthalpy of formation from the elements in their standard reference states in J·mol <sup>-1</sup> .
ΔG <sub>f</sub> <sup>°</sup>	Gibbs free energy of formation from the elements in their reference states in J·mol <sup>-1</sup> .
K <sub>f</sub>	Equilibrium constant of formation.
R	Gas constant, 8.3143 ± 0.0008 J·K <sup>-1</sup> ·mol <sup>-1</sup> .
F	Faraday constant, 96,487.0 ± 1.0 J·V <sup>-1</sup> ·mol <sup>-1</sup> .
A	Avogadro's number, (6.022094 ± 0.000008) × 10 <sup>23</sup> mol <sup>-1</sup> .
log	Common logarithm, base 10.
ln	Natural logarithm, base e = 2.71828 . . .
V	Volt.

Values for the gas constant (R) and the Faraday constant (F) used in the calculations are those adopted by the CODATA Task Group (1976), although their values differ slightly from the most recent least-squares evaluation of the physical constants by Cohen and Taylor (1973). For Avogadro's number (used in calculating molar volumes from X-ray cell dimensions), we have used the value of Deslattes and others (1974) 6.022094 ± 0.000008 × 10<sup>23</sup> mol<sup>-1</sup>.

For convenience, we also give values for the atomic weights for 1975 (scale C<sup>12</sup> = 12.000) (Commission on Atomic Weights, 1976) in alphabetical order by their chemical symbol in table 2.

## REFERENCE STATES AND TRANSITIONS

The reference states for ΔH<sub>f</sub><sup>°</sup>, ΔG<sub>f</sub><sup>°</sup>, and log K<sub>f</sub> of the compounds are the elements in their standard states at 1 bar pressure (10<sup>5</sup> pascals) and the



## THERMODYNAMIC PROPERTIES OF MINERALS

TABLE 2.—Atomic weights for 1975

Element	Symbol	Atomic weight	Element	Symbol	Atomic weight
Actinium	Ac	227.0278	Sodium	Na	22.98977
Silver	Ag	107.868	Niobium	Nb	92.9064
Aluminum	Al	26.98154	Neodymium	Nd	144.24
Americium	Am	(243)	Neon	Ne	20.179
Argon	Ar	39.948	Nickel	Ni	58.70
Arsenic	As	74.9216	Neptunium	Np	237.0482
Astatine	At	(210)	Oxygen	O	15.9994
Gold	Au	196.9665	Osmium	Os	190.2
Boron	B	10.81	Phosphorus	P	30.97376
Barium	Ba	137.33	Protactinium	Pa	231.0359
Beryllium	Be	9.01218	Lead	Pb	207.2
Bismuth	Bi	208.9804	Palladium	Pd	106.4
Bromine	Br	79.904	Polonium	Po	(209)
Carbon	C	12.011	Promethium	Pm	(145)
Calcium	Ca	40.08	Praseodymium	Pr	140.9077
Cadmium	Cd	112.41	Platinum	Pt	195.09
Cerium	Ce	140.12	Plutonium	Pu	(244)
Chlorine	Cl	35.453	Radium	Ra	226.0254
Cobalt	Co	58.9332	Rubidium	Rb	85.4678
Chromium	Cr	51.996	Rhenium	Re	186.207
Cesium	Cs	132.9054	Rhodium	Rh	102.9055
Copper	Cu	63.546	Radon	Rn	(222)
Dysprosium	Dy	162.50	Ruthenium	Ru	101.07
Erbium	Er	167.26	Sulfur	S	32.06
Europium	Eu	151.96	Antimony	Sb	121.75
Fluorine	F	18.9984	Scandium	Sc	44.9559
Iron	Fe	55.847	Selenium	Se	78.96
Francium	Fr	(223)	Silicon	Si	28.0855
Gallium	Ga	69.72	Samarium	Sm	150.4
Gadolinium	Gd	157.25	Tin	Sn	118.69
Germanium	Ge	72.59	Strontium	Sr	87.62
Hydrogen	H	1.0079	Tantalum	Ta	180.9479
Helium	He	4.0026	Terbium	Tb	158.9254
Hafnium	Hf	178.49	Technetium	Tc	(97)
Mercury	Hg	200.59	Tellurium	Te	127.60
Holmium	Ho	164.9304	Thorium	Th	232.0381
Iodine	I	126.9045	Titanium	Ti	47.90
Indium	In	114.82	Thallium	Tl	204.37
Iridium	Ir	192.22	Thulium	Tm	168.9342
Potassium	K	39.0983	Uranium	U	238.029
Krypton	Kr	83.80	Vanadium	V	50.9414
Lanthanum	La	138.9055	Tungsten	W	183.85
Lithium	Li	6.941	Xenon	Xe	131.30
Lutetium	Lu	174.97	Yttrium	Y	88.9059
Magnesium	Mg	24.305	Ytterbium	Yb	173.04
Manganese	Mn	54.9380	Zinc	Zn	65.38
Molybdenum	Mo	95.94	Zirconium	Zr	91.22
Nitrogen	N	14.0067			

stated temperature. The standard states for the condensed elements are the most stable form at 1 bar pressure and the stated temperature. For gaseous elements, the standard state is the ideal gas at 1 bar pressure. The reference pressure for the standard state adopted for these tables is the bar, that is,  $10^5$  pascals. The reasons for this choice are:

- In most modern high-pressure—high-temperature equilibrium studies on minerals, the pressure is measured in bars.
- The use of the bar as the standard pressure in conjunction with the joule for energy (or work) simplifies conversion of the  $Pv$  term ( $\text{cm}^3 \cdot \text{bar}$ ) in high-pressure calculations of mineral equilibria. Thus,  $1 \text{ joule} = 10.0 \text{ cm}^3 \cdot \text{bar}$  in contrast with  $1 \text{ calorie} = 41.2929 \text{ cm}^3 \cdot \text{atm}$  in terms of older (non-SI) units.
- The *standard atmosphere* used as the reference pressure for most thermochemical measurements, with the frequent exception of the  $PvT$  properties of gases, is an arbitrarily adopted unit. In terms of the SI base unit of pressure, the *standard atmosphere* is equal to 101325 pascals.
- The effect of the change of reference pressure from 1 atmosphere, as used in an earlier edition of these tables (Robie and Waldbaum, 1968), to the present choice of 1 bar has an insignificant effect upon the tabulated values of the thermodynamic functions for the condensed phases and only a minor and constant effect for the gas phases.

All data listed in these tables have been corrected to the standard state  $P=1$  bar. For a condensed phase (liquid or solid), it can be readily shown that the effect of changing the reference state from 1 atmosphere to 1 bar has only a trivial effect upon all the thermodynamic properties tabulated in this report *except* for  $\Delta G_f^\circ$ .

For a gaseous phase, the reference state is the ideal gas, that is, one that obeys the equation of state  $Pv=RT$ . From the equation of state, it follows that:

$$v = RT/P$$

from which

$$(\partial v / \partial T)_P = R/P, \text{ and } (\partial^2 v / \partial T^2)_P = 0,$$

Then from standard thermodynamic relations

$$(\partial C_P / \partial P)_T = T(\partial^2 v / \partial T^2)_P = 0$$

and

$$(\partial S / \partial P)_T = -(\partial v / \partial T)_P = -R/P$$

from which

$$dS = -(R/P)dP$$

For the change in pressure from  $P=1$  atm (1.0135 bar) to 1.000 bar

$$\Delta S = -R \int_{1.013}^{1.000} (1/P)dP = 0.11 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$$

Also, for an ideal gas,

$$dH = TdS + vdP = T(-R/P) dP + (RT/P)dP = 0.$$

Thus, for a gaseous phase,  $C_p^\circ$ ,  $(H_T^\circ - H_{298}^\circ)/T$ , and  $\Delta H_f^\circ$  are independent of pressure, but the numerical values of  $S^\circ$ ,  $\Delta G_f^\circ$ , and  $(G_T^\circ - H_{298}^\circ)/T$  depend upon the choice of pressure. Similarly it can be shown that the change of the standard state from a pressure of 1 atmosphere to 1 bar does not affect the enthalpy of formation (from the elements in their reference states) but will cause a change in the Gibbs free energy of formation of a condensed phase if and only if one of the reference elements (usually oxygen) is a gas.

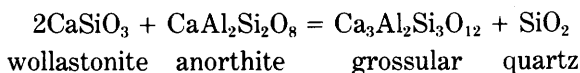
The entropies of the gaseous elements and compounds were converted to the standard state  $P=1$  bar, using the above relations, before entering the various thermodynamic data into the data bank. Inasmuch as the computer program calculates  $\Delta G_{f,T}^\circ$  from  $\Delta H_f^\circ$  and the entropies or Gibbs energy functions of the constituent elements, the values of  $\Delta G_{f,T}^\circ$  are automatically corrected to the 1 bar standard state.

The National Bureau of Standards Technical Note 270 series, the JANAF thermochemical tables, and the CODATA tables have retained the use of the *standard atmosphere* as the reference pressure. The authors hope that in the near future the General Conference of Weights and Measures of the International Bureau of Weights and Measures will recommend the elimination of the standard atmosphere as the reference pressure.

Data are listed for the elements in their standard reference states, and for a few in nonstandard states; for example,  $S_2$  gas and the diamond form of carbon. Melting and boiling points and their associated enthalpy changes are listed at the bottom of each table of high-temperature properties. A horizontal dashed line in the tables indicates a transition in the phase. A dashed line in the columns  $\Delta H_f^\circ$ ,  $\Delta G_f^\circ$ , and  $\log K_f$ , indicates a transition in one of the reference elements. Transitions in the reference elements are also listed separately at the bottom of each table. Inasmuch as most of the high-temperature "heat-capacity" data are actually heat-content measurements and not true heat capacities ( $C_p^\circ$ ), we have followed the practice of Kelley (1960) and have treated all the high-temperature transitions as first order at a single temperature. At the transition temperature, the functions  $(H_T^\circ - H_{298}^\circ)/T$ ,  $S_T^\circ$ , and  $\Delta H_{f,T}^\circ$  make a stepwise change;  $\Delta G_{f,T}^\circ$  and  $(G_T^\circ - H_{298}^\circ)/T$ , are continuous, but their temperature derivatives change abruptly. For those elements (and their compounds) for which we have, of necessity, adopted a nonequilibrium phase as the reference state (for example,  $S_2$  gas above 716.9 K), there will also be a discontinuity in both  $\Delta G_{f,T}^\circ$  and  $(G_T^\circ - H_{298}^\circ)/T$  at the transition temperature. These properties of the functions must be borne in mind when interpolating in the tables.

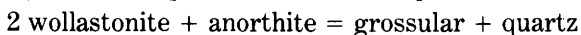
The reference state adopted for an element above its normal boiling or sublimation temperature is not necessarily its equilibrium state. Thus, at equilibrium, liquid sulfur boils at 1 bar pressure and approximately 716.9 K to a gas composed of S, S<sub>2</sub>, S<sub>4</sub>, S<sub>6</sub>, S<sub>8</sub>, etc., but for our reference table, we have assumed the gas phase to be only S<sub>2</sub>. In these ambiguous cases, we have chosen either the dominant species in the gas or that species for which the best thermodynamic data are available as the reference state.

Enthalpies and Gibbs free energies of formation for multiple-oxide phases using the *binary oxides* as reference states have also been computed and tabulated, inasmuch as many mineralogical equilibria involve only binary or multiple-oxide phases; for example:



and because the enthalpies of formation of most multiple-oxide phases are determined using the binary oxides as the reactants. Tables of the thermodynamic functions for temperatures above 298.15 K for multiple-oxide phases calculated using the *binary oxides* as the reference phases immediately follow the appropriate table calculated from the elements and are differentiated by the heading "FORMATION FROM THE OXIDES" above the columns for  $\Delta H_f^\circ$ ,  $\Delta G_f^\circ$ , and  $\log K_f$  and by asterisks immediately to the right of the entries for  $\Delta H_f^\circ$  and  $\Delta G_f^\circ$ .

When using the binary oxides as the reference states, one must remember that in this convention,  $\Delta H_f^\circ$  and  $\Delta G_f^\circ$  for these reference oxides are zero at all temperatures. For example,  $\Delta G_{1000}^\circ$  for the reaction



may be calculated from either the tabulated values of  $\Delta G_{f,1000}^\circ$  (elements as reference states), or  $\Delta G_{1000}^\circ$  (oxides as reference states) for each of the phases in the above reaction. Thus:

$$\Delta G_{1000}^\circ (\text{oxides}) = \{[-304.53 + 0] - [-136.25 + 2(-91.18)]\} = 14.08 \text{ kJ}$$

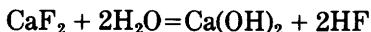
or

$$\Delta G_{1000}^\circ (\text{elements}) = \{[-5448.79 + (-729.98)] - [-3488.51 + 2(-1352.17)]\} = 14.08 \text{ kJ}$$

Both calculations must obviously give the same result within the rounding error. However, in estimating the uncertainty in the resulting value of  $\Delta G_f^\circ$  for a reaction involving only oxide phases, one should use the uncertainties associated with the  $\Delta G_f^\circ$  values calculated from the oxides, inasmuch as this value usually corresponds more closely to the actual calorimetric reaction scheme from which the individual  $\Delta G_f^\circ$  values were obtained.

The user is cautioned not to mix values of  $\Delta G_f^\circ$  calculated from the elements for one phase with those obtained from the oxides for another in calculating  $\Delta G_f^\circ$  of a reaction involving the two phases, because a mean-

ingless result ensues. If a reaction involves both multiple-oxide phases and nonoxide phases, as in



fluorite steam portlandite

$\Delta G_T^\circ$  for the reaction must be calculated using *only* values from the tabulated values of  $\Delta G_{f,T}^\circ$  calculated from the elements.

### SOURCES OF DATA

Many critical evaluations of thermochemical data have been particularly helpful in constructing these tables. For the thermodynamic functions of the elements at high temperatures, we have adopted the values selected by Hultgren and others (1973). The CODATA (1976) key values have been adopted when they differed significantly from those of Hultgren and others (1973). For the sulfides, arsenides, tellurides, selenides, and sulfosalts, the summaries by Mills (1974) and by Barton and Skinner (1977) have been very helpful. The tabulations by Kelley (1960) and by Kelley and King (1961) were particularly useful as a source of the pre-1960 heat-content and heat-capacity data. We have also relied heavily upon the critical evaluations of the National Bureau of Standards Technical Note 270 series (Wagman and others, 1968, 1969, 1971; Parker and others, 1971; Schumm and others, 1973) and of the JANAF thermochemical tables (Stull and Prophet, 1971; Chase and others, 1974, 1975).

In evaluating the data for the silicates, we have accepted the revised values for  $\Delta H_f^\circ$  for those silicates given by Hemingway and Robie (1977), which include corrections for the effect of the particle size of quartz and for the incorrect value of  $\Delta H_f^\circ$  of gibbsite ( $\text{Al}(\text{OH})_3$ ) used in earlier HF solution calorimetry studies. For those aluminum silicates for which definitive structural evidence of Al/Si disorder was available we have corrected the  $S_{298}^\circ$  values for the configurational terms, that is,  $S_0^\circ \neq 0$ , arising from frozen-in Al/Si disorder at 0 K, using the summary of Ulbrich and Waldbaum (1976) as a guide. We have also added a correction to the entropy of several manganese and iron compounds for which the accepted value of  $S_{298}^\circ$  was based upon measurements of the heat capacity only above 50 K and for which other evidence indicated the existence of an unextracted magnetic contribution to  $S_{298}^\circ$  below 50 K (see, for example, Robie, 1965, or Ulbrich and Waldbaum, 1976).

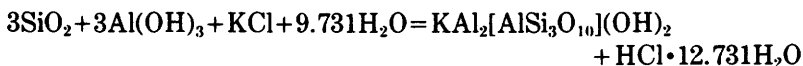
Values for the thermodynamic properties at 298.15 K for the more common aqueous ions are also listed in order to facilitate calculations of aqueous equilibria. The reference state for the free energies of the aqueous ions is the hypothetical ideal solution of unit molality. Values for  $\Delta G_f^\circ$  are listed on the basis of the usual convention that  $\Delta G_f^\circ$ ,  $\Delta H_f^\circ$ ,  $S^\circ$ , and  $C_p^\circ$  are identically 0 for aqueous  $\text{H}^+$  ion in the hypothetical 1 molal ideal solution. A more complete discussion of the conventions adopted for



tabulating the thermodynamic properties of aqueous ions has been given by F. D. Rossini (1950, *Chemical thermodynamics*: New York, John Wiley, p. 320–370).

The molar volumes of the condensed phases are principally from the summary by Robie and others (1967), augmented by more recent precise X-ray measurements of unit-cell parameters. Although our principal sources of data for  $\Delta H_f^\circ$ , or  $\Delta G_f^\circ$ , have been solution or combustion calorimetry, for many compounds the best available data are values of  $\Delta G_f^\circ$ , calculated from solubilities, electrochemical cells, reduction equilibria, or decomposition pressure data; we have used these equilibrium studies to supplement the calorimetric data whenever possible. For the simpler gases, the thermodynamic constants calculated from spectroscopic data are usually the most precise.

In order to insure internal consistency in these tables and because of the complex nature of many of the reaction schemes used to obtain  $\Delta H_f^\circ$ , or  $\Delta G_f^\circ$ , we have corrected all the older data to the values adopted here. For multiple-oxide compounds, the heats of formation are most commonly measured utilizing the binary oxides as reference phases. However, stoichiometric  $K_2O$  cannot be prepared reproducibly, and  $FeO$  is thermodynamically unstable. Furthermore,  $\alpha-Al_2O_3$ , corundum, is insoluble in all common aqueous calorimetric solvents. Consequently, mixed sets of reactants such as the alkali halides, aluminum hydroxide (gibbsite), or an element have frequently been used as the reference phases in HF solution calorimetry for determining  $\Delta H_f^\circ$  of aluminosilicates. For example, Barany (1964) measured the enthalpy change for the reaction



and by utilizing literature data for the enthalpies of formation of the other phases, he calculated  $\Delta H_{f,298}^\circ$  for muscovite. Accordingly, any improvement of  $\Delta H_f^\circ$  of quartz, gibbsite, sylvite, or aqueous  $HCl$  would alter the enthalpy of formation of muscovite. Recent measurements of  $\Delta H_{f,298}^\circ$  of gibbsite by Hemingway and Robie (1977) have shown that the value of  $\Delta H_{f,298}^\circ$  of gibbsite used by Barany (1964) to calculate the enthalpy of formation of muscovite was in error by  $11230 J \cdot mol^{-1}$ , and accordingly we have corrected Barany's (1964) calorimetric value for  $\Delta H_{f,298}^\circ$  of muscovite, and also several other aluminosilicates for which gibbsite was one of the reactants, to accord with this new  $\Delta H_{f,298}^\circ$  of gibbsite.

### METHODS OF CALCULATION

Having chosen what we believe are the currently "best available" values for  $H_T^\circ - H_{298}^\circ$ , or  $C_P^\circ(T)$ ,  $S_{298}^\circ$ , and either  $\Delta H_{f,298}^\circ$  or  $\Delta G_{f,298}^\circ$ , we have calculated the Gibbs free energy function, and the enthalpy, free energy, and the equilibrium constant of formation at 100 K intervals using the following relations:

$$(G_T^\circ - H_{298}^\circ)/T = (H_T^\circ - H_{298}^\circ)/T - S_T^\circ \quad (1)$$

$$\Delta H_{f,T}^\circ = \Delta H_{f,298}^\circ + \Delta(H_T^\circ - H_{298}^\circ) \quad (2)$$

$$\Delta G_{f,T}^\circ = \Delta H_{f,298}^\circ + T\Delta[(G_T^\circ - H_{298}^\circ)/T] \quad (3)$$

and

$$\log K_{f,T} = -\Delta G_{f,T}^\circ/2.30258 RT = -\Delta G_{f,298}^\circ/19.1444T \quad (4)$$

These values together with  $C_p^\circ$ ,  $S_T^\circ$  and  $(H_T^\circ - H_{298}^\circ)/T$  are tabulated in the second section.

A Fortran IV program was used for the above calculations. The essential feature of the program is that internally consistent thermodynamic functions can be calculated for several hundred compounds in a single run of the computer. This consistency is accomplished by first calculating the thermodynamic functions for the reference elements and oxides and then holding these data in storage for later computations involving substances having these elements or oxides as reference phases. As new thermodynamic data become available, only a minimum number of changes in the data base are needed to prepare a completely revised set of internally consistent tables.

The input data supplied to the computer are the identifying name of the substance, the entropy, the enthalpy, and Gibbs free energy of formation at 298.15 K and their uncertainties, and the entropy and enthalpy increments,  $S_T^\circ - S_{298}^\circ$  and  $H_T^\circ - H_{298}^\circ$ , at 100 K intervals, together with the number of atoms of each element in the chemical formula. Auxiliary data such as the melting and boiling points and enthalpies of melting and vaporization are also included. The program computes the formula weight of the compound on the basis of the atomic weights of the elements (1975 scale) and values for  $S_T^\circ$ ,  $\Delta H_{f,T}^\circ$ ,  $\Delta G_{f,T}^\circ$ ,  $\log K_{f,T}$ ,  $C_p^\circ$ ,  $(H_T^\circ - H_{298}^\circ)/T$ , and  $(G_T^\circ - H_{298}^\circ)/T$  at 100 K intervals up to 1,800 K.

Although the absolute value of  $\Delta G_{f,T}^\circ$  or  $\Delta H_{f,T}^\circ$  of the more complex compounds is rarely known more accurately than  $\pm 1,000$  joules, these quantities are tabulated to the nearest 10 joules. This procedure is justified because the temperature derivatives of  $\Delta G_f^\circ$  and  $\Delta H_f^\circ$ ,

$$(d\Delta G_f^\circ/dT)_p = -\Delta S_f^\circ \quad (5)$$

and

$$(d\Delta H_f^\circ/dT)_p = \Delta C_p^\circ \quad (6)$$

are calculated from the heat-content data, which are known independently of the enthalpy or Gibbs free energy of formation. The practice of rounding tabulated values of  $\Delta G_f^\circ$  or  $\Delta H_f^\circ$  on the basis of the uncertainty in the absolute value does not utilize the full accuracy of the heat-capacity information and destroys the necessary internal consistency between  $\Delta H_{f,298}^\circ$  and the Gibbs free-energy function (eq. 3). Furthermore, in many instances, the *differences* between  $\Delta H_f^\circ$  or  $\Delta G_f^\circ$  for polymorphs are often known more accurately from phase-equilibria or calorimetric investigations than are the individual  $\Delta H_f^\circ$  or  $\Delta G_f^\circ$  values for a phase, so that

rounding off again tends to obscure small differences of major importance in calculations of geological interest.

The uncertainties assigned to the properties apply only to the values at 298.15 K and were taken principally from the original sources of experimental data. By convention, the uncertainty interval reported for calorimetric measurements is twice the standard deviation of the mean (Rossini, 1956, p. 319); that is,

$$\delta = 2[\sum(x_i - \bar{x})^2/n(n-1)]^{1/2} \quad (7)$$

where  $x_i$  is the value for an individual measurement,  $\bar{x}$  is the arithmetic mean of all the measurements, and  $n$  is the number of observations.

For substances where  $\Delta H_{f,298}^\circ$  is the directly measured quantity, the free energy was calculated from

$$\Delta G_{f,298}^\circ = \Delta H_{f,298}^\circ - 298.15\Delta S_{f,298}^\circ \quad (8)$$

and the uncertainty in the free energy was calculated from

$$\sigma_G = [(\sigma_H)^2 + (298\sigma_S)^2 + \sum(298n_i\sigma_{S_i})^2]^{1/2} \quad (9)$$

where  $\sigma_S$  is the uncertainty in the entropy of the substance, the  $\sigma_{S_i}$  are the uncertainties in the entropies of the  $i$  reference elements, and the  $n_i$  are the number of moles of each element in the chemical formula of the substance. Uncertainties derived in this manner were rounded upward to the nearest 10 joules.

For substances in which  $\sigma_G$  is less than  $\sigma_H$ , the basic quantities used in the calculation were  $\Delta G_{f,298}^\circ$  and  $\sigma_G$  derived from electrochemical cell measurements, solubilities, or phase-equilibrium data. Hence,  $\Delta H_{f,298}^\circ$  is a more indirectly derived quantity having a larger uncertainty. For these substances,  $\sigma_H$  was calculated from

$$\sigma_H = [(\sigma_G)^2 + (298\sigma_S)^2 + \sum(298n_i\sigma_{S_i})^2]^{1/2} \quad (10)$$

Camera-ready copy of the tables of the thermodynamic properties, and of the bibliography, were prepared from the output file (tape) of the FORTRAN IV program, using the WYLBUR text editor and the extended print facility at the Computer Center of the National Institutes of Health.

Several of the tables in the second section are incomplete because of the lack of adequate data on the enthalpies of formation or entropies at 298.15 K of these substances. The tables are nonetheless included, so that when such data become available, one may readily calculate the remaining functions using equations 2, 3, and 4 given above, or use equilibrium data and the third-law method to obtain the standard state enthalpy or Gibbs free energy change for the reaction ( $\Delta H_r^\circ$ , or  $\Delta G_r^\circ$ ), following the procedures illustrated, for example, by Robie (1965).

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References S $\Delta H_{f,298}^0$ $\Delta G_{f,298}^0$ $C_p^0$
ELEMENTS							
SILVER (REFERENCE STATE) Ag	107.868	42.55 0.21	10.272 0.002	0	0	0 107	107
Ag <sup>+</sup> AQUEOUS ION STD. STATE, n = 1	107.868	73.38 0.40		105750 85	77077 100	-13.504 0.018	35 35
ALUMINIUM (REFERENCE STATE) Al	26.982	28.35 0.08	9.999 0.001	0	0	0 107	107
Al <sup>+++</sup> AQUEOUS ION STD. STATE, n = 1	26.982	-308.00 15.00		-531000 4000	-489400 1400	85.741 0.245	94 94
ARGON (REFERENCE STATE) Ar (IDEAL GAS)	39.948	154.84 0.02	24789.2 3.4	0	0	0 107	107
ARSENIC (REFERENCE STATE) As	74.922	35.69 0.84	12.963 0.015	0	0	0 107	107
GOLD (REFERENCE STATE) Au	196.966	47.49 0.21	10.215 0.002	0	0	0 107	107
BORON (REFERENCE STATE) B	10.810	5.90 0.08	4.386 0.007	0	0	0 107	107
BARIUM (REFERENCE STATE) Ba	137.340	62.42 0.84	38.21 0.02	0	0	0 107	107
Ba <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	137.340	9.60 0.85		-537640 120	-560740 120	98.240 0.021	214 214
BERYLLIUM (REFERENCE STATE) Be	9.012	9.54 0.08	4.880 0.002	0	0	0 107	107
Be <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	9.012	-130.00 0.85		-383000 850	-379700 850	66.522 0.149	214 214
BISMUTH (REFERENCE STATE) Bi	208.980	56.74 0.42	21.309 0.011	0	0	0 107	76
Bi <sup>+++</sup> AQUEOUS ION STD. STATE, n = 1	208.980				82800 850	-14.506 0.149	262
BROMINE (REFERENCE STATE) Br <sub>2</sub> (LIQUID)	159.808	152.32 0.04	54.58 0.20	0	0	0 107	107
BROMINE (IDEAL GAS) Br <sub>2</sub>	159.808	245.46 0.05	24789.2 3.4	30910 200	3140 300	-0.550 0.053	35 35 107
Br <sup>-</sup> AQUEOUS ION STD. STATE, n = 1	79.904	82.84 0.20		-121500 150	-104010 170	18.222 0.030	35 35
CARBON (REFERENCE STATE) C	12.011	5.74 0.01	5.298 0.001	0	0	0 107	107
DIAMOND C	12.011	2.38 0.01	3.417 0.001	1895 42	2900 84	-0.508 0.015	107 87 107
CALCIUM (REFERENCE STATE) Ca	40.080	41.63 0.42	26.19 0.04	0	0	0 107	107
Ca <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	40.080	-53.10 2.00		-542830 1200	-553540 1200	96.978 0.021	214 214
CADMIUM (REFERENCE STATE) Cd	112.400	51.80 0.17	13.005 0.003	0	0	0 107	107
Cd <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	112.400	-73.20 0.85		-75900 120	-77580 120	13.592 0.021	262 262
CERIUM (REFERENCE STATE) Ce	140.120	69.46 8.37	20.77 0.02	0	0	0 107	107
Ce <sup>+++</sup> AQUEOUS ION STD. STATE, n = 1	140.120	-205.00 5.00		-696200 850	-672000 850	117.732 0.149	262 262
Ce <sup>++++</sup> AQUEOUS ION STD. STATE, n = 1	140.120	-301.00 5.00		-537200 850	-503800 850	88.264 0.149	262 262
CHLORINE (REFERENCE STATE) Cl <sub>2</sub> (IDEAL GAS)	70.906	223.08 0.04	24789.2 3.4	0	0	0 107	107
Cl <sup>-</sup> AQUEOUS ION STD. STATE, n = 1	35.453	56.73 0.16		-167080 88	-131270 110	22.999 0.019	35 35

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References $\Delta H_{f,298}^0$ $\Delta G_{f,298}^0$ S	$C_p^0$
ELEMENTS								
COBALT (REFERENCE STATE) Co	58.933	30.04 0.42	6.670 0.002	0	0	0 107	107	
Co <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	58.933	-113.00 5.00		-58200 500	-54400 500	9.531 0.088	263 263	
Co <sup>+++</sup> AQUEOUS ION STD. STATE, n = 1	58.933	-305.00 5.00		92000 5000	134000 5000	-23.476 0.876	263 263	
CHROMIUM (REFERENCE STATE) Cr	51.996	23.64 0.21	7.231 0.001	0	0	0 107	107	
Cr <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	51.996			-144000 1000			263	
CESIUM (REFERENCE STATE) Cs	132.905	85.23 0.40	69.73 0.10	0	0	0 107	107	
Cs <sup>+</sup> AQUEOUS ION STD. STATE, n = 1	132.905	132.84 0.40		-258040 130	-283625 150	49.690 0.026	35 35	
COPPER (REFERENCE STATE) Cu	63.546	33.15 0.08	7.113 0.003	0	0	0 107	107	
Cu <sup>+</sup> AQUEOUS ION STD. STATE, n = 1	63.546	41.00 0.42		71670 100	50000 100	-8.760 0.018	263 263	
Cu <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	63.546	-99.60 0.42		64770 100	65520 100	-11.479 0.018	263 263	
DYSPROSIUM (REFERENCE STATE) Dy	162.500	74.89 0.84	19.01 0.02	0	0	0 107	107	
ERBIUM (REFERENCE STATE) Er	167.260	73.18 0.15		0	0	0 107	107	
EUROPIUM (REFERENCE STATE) Eu	151.960	80.79 0.16	28.97 0.02	0	0	0 107	107	
FLUORINE (REFERENCE STATE) F <sub>2</sub> (IDEAL GAS)	37.997	202.79 0.04	24789.2 3.4	0	0	0 107	107	
F <sup>-</sup> AQUEOUS ION STD. STATE, n = 1	18.998	-13.18 0.54		-335350 650	-281705 670	49.354 0.117	35 35	
IRON (REFERENCE STATE) Fe	55.847	27.28 0.13	7.092 0.004	0	0	0 107	107	
Fe <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	55.847	-138.00 0.85		-89100 1000	-78870 1000	13.818 0.021	263 263	
Fe <sup>+++</sup> AQUEOUS ION STD. STATE, n = 1	55.847	-316.00 0.85		-48500 1000	-4600 1000	0.806 0.021	263 263	
GALLIUM (REFERENCE STATE) Ga	69.720	40.83 0.21	11.79 0.01	0	0	0 107	107	
GADOLINIUM (REFERENCE STATE) Gd	157.250	68.45 1.25	19.89 0.02	0	0	0 107	107	
GERMANIUM (REFERENCE STATE) Ge	72.590	31.09 0.21	13.63 0.005	0	0	0 107	107	
HYDROGEN (REFERENCE STATE) H <sub>2</sub> (IDEAL GAS)	2.016	130.68 0.04	24789.2 3.4	0	0	0 107	107	
H <sup>+</sup> AQUEOUS ION STD. STATE, n = 1	1.008			0	0	0 35 35		
HELIUM (REFERENCE STATE) He (IDEAL GAS)	4.003	126.15 0.01	24789.2 3.4	0	0	0 107	107	
HAFNIUM (REFERENCE STATE) Hf	178.490	43.56 0.21	13.479 0.010	0	0	0 107	107	
MERCURY (REFERENCE STATE) Hg (LIQUID)	200.590	75.90 0.08	14.822 0.002	0	0	0 107	107	
Hg <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	200.590	-32.00 0.85		171000 850	164400 120	-28.802 0.021	263 263	
Hg <sub>2</sub> <sup>++</sup> AQUEOUS ION STD. STATE, n = 1	401.180	84.56 0.85		172000 850	153600 120	-26.910 0.021	263 263	



Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume cm <sup>3</sup>	$\Delta H_f^0, 298$ J/mol	$\Delta G_f^0, 298$ J/mol	Log $K_f$	References $\Delta H_f^0$ S $\Delta G_f^0$	$\Delta H_f^0$ S $\Delta G_f^0$	$\Delta H_f^0$ S $\Delta G_f^0$
ELEMENTS									
HOLMIUM (REFERENCE STATE) Ho	164.930	75.02 1.67	18.74 0.01	0	0	0	107	107	
IODINE (REFERENCE STATE) I <sub>2</sub>	253.809	116.15 0.08	51.29 0.06	0	0	0	107	107	
IODINE I <sub>2</sub> (IDEAL GAS)	253.809	260.68 0.06	24789.2 3.4	62420 80	19329 80	-3.386 0.001	32	32	107
I <sup>-</sup> AQUEOUS ION STD. STATE, $\mu = 1$	126.905	106.70 0.20		-56900 840	-51915 860	9.096 0.151	35	35	
INDIUM (REFERENCE STATE) In	114.820	57.84 0.84	15.753 0.005	0	0	0	107	107	
IRIDIUM (REFERENCE STATE) Ir	192.220	35.48 0.17	8.519 0.005	0	0	0	107	107	
POTASSIUM (REFERENCE STATE) K	39.098	64.68 0.20	45.36 0.09	0	0	0	107	107	
K <sup>+</sup> AQUEOUS ION STD. STATE, $\mu = 1$	39.098	101.04 0.25		-252170 100	-282490 120	49.492 0.021	35	35	
KRYPTON (REFERENCE STATE) Kr (IDEAL GAS)	83.800	164.08 0.02	24789.2 3.4	0	0	0	107	107	
LANTHANUM (REFERENCE STATE) La	138.906	56.90 2.51	22.47 0.01	0	0	0	107	107	
LITHIUM (REFERENCE STATE) Li	6.940	29.12 0.02	13.017 0.007	0	0	0	107	107	
Li <sup>+</sup> AQUEOUS ION STD. STATE, $\mu = 1$	6.941	11.30 0.35		-278455 90	-292620 110	51.267 0.019	35	35	
LUTETIUM (REFERENCE STATE) Lu	174.970	50.96 0.84	17.77 0.01	0	0	0	107	107	
MAGNESIUM (REFERENCE STATE) Mg	24.305	32.68 0.13	13.996 0.007	0	0	0	107	107	
Mg <sup>++</sup> AQUEOUS ION STD. STATE, $\mu = 1$	24.305	-138.00 4.20		-466850 840	-454800 1670	79.679 0.149	214	214	
MANGANESE (REFERENCE STATE) Mn	54.938	32.01 0.08	7.354 0.007	0	0	0	107	107	
Mn <sup>++</sup> AQUEOUS ION STD. STATE, $\mu = 1$	54.938	-73.60 0.85		-220760 120	-228000 850	39.945 0.149	263	263	
MOLYBDENUM (REFERENCE STATE) Mo	95.940	28.66 0.21	9.387 0.005	0	0	0	107	107	
NITROGEN (REFERENCE STATE) N <sub>2</sub> (IDEAL GAS)	28.013	191.61 0.02	24789.2 3.4	0	0	0	107	107	
SODIUM (REFERENCE STATE) Na	22.990	51.30 0.02	23.812 0.010	0	0	0	107	107	
Na <sup>+</sup> AQUEOUS ION STD. STATE, $\mu = 1$	22.990	58.41 0.20		-240360 65	-261900 85	45.884 0.015	35	35	
NIOBIUM (REFERENCE STATE) Nb	92.906	36.40 0.42	10.828 0.005	0	0	0	107	107	
NEODYMIUM (REFERENCE STATE) Nd	144.240	71.09 4.18	20.57 0.01	0	0	0	107	107	
NEON (REFERENCE STATE) Ne (IDEAL GAS)	20.179	146.32 0.02	24789.2 3.4	0	0	0	107	107	
NICKEL (REFERENCE STATE) Ni	58.700	29.87 0.08	6.588 0.003	0	0	0	107	107	
Ni <sup>++</sup> AQUEOUS ION STD. STATE, $\mu = 1$	58.700	-129.00 0.85		-54000 850	-45600 850	7.989 0.149	263	263	
OXYGEN (REFERENCE STATE) O <sub>2</sub> (IDEAL GAS)	31.999	205.15 0.04	24789.2 3.4	0	0	0	35	107	
OSMIUM (REFERENCE STATE) Os	190.200	32.64 0.06	8.423 0.005	0	0	0	107	107	
PHOSPHORUS (REFERENCE STATE) P	30.974	22.85 0.08	17.2 0.3	0	0	0	107	107	

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol $\cdot$ K	Molar volume cm $^3$	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References		
							S	$\Delta H_f^0$	$\Delta G_f^0$
ELEMENTS									
LEAD (REFERENCE STATE) Pb	207.200	65.06 0.42	18.267 0.086	0	0	0 107			107
Pb $^{2+}$ AQUEOUS ION STD. STATE, $\nu = 1$	207.200	10.00 0.85		-1700 850	-24400 .120	4.275 262 0.021	262		262
PALLADIUM (REFERENCE STATE) Pd	106.400	37.82 0.21	8.862 0.005	0	0	0 107			107
PRASEODYMIUM (REFERENCE STATE) Pr	140.908	73.93 4.18	20.80 0.01	0	0	0 107			107
PLATINUM (REFERENCE STATE) Pt	195.090	41.63 0.21	9.091 0.004	0	0	0 107			107
PLUTONIUM (REFERENCE STATE) Pu	244.002	51.46 8.37	12.04 0.01	0	0	0 107			107
RUBIDIUM (REFERENCE STATE) Rb	85.468	76.78 0.30	55.85 0.10	0	0	0 107			107
Rb $^+$ AQUEOUS ION STD. STATE, $\nu = 1$	85.468	120.46 0.40		-251120 130	-291715 150	51.108 0.026	35		35
RHENIUM (REFERENCE STATE) Re	186.207	36.53 0.38	8.860 0.004	0	0	0 107			107
RHODIUM (REFERENCE STATE) Rh	102.906	31.54 0.21	8.282 0.002	0	0	0 107			107
RADON (REFERENCE STATE) Rn (IDEAL GAS)	222.000	176.23 0.00	24789.2 3.3	0	0	0 107			107
RUTHENIUM (REFERENCE STATE) Ru	101.070	28.53 0.21	8.171 0.004	0	0	0 107			107
SULFUR (REFERENCE STATE) S	32.060	31.80 0.21	15.511 0.005	0	0	0 107			107
S $^{2-}$ AQUEOUS ION STD. STATE, $\nu = 1$	32.060	-15.00 0.85		33000 850	85000 850	-15.032 0.149	262		262
DIATOMIC SULFUR S $_2$ (IDEAL GAS)	64.120	228.17 0.05	24789.2 3.4	128400 500	79453 669	-13.920 0.117	107		107
OCTA-ATOMIC SULFUR S $_8$ (IDEAL GAS)	256.480	430.32 1.67	24789.2 3.4	101250 630	48835 920	-8.556 0.161	107		107
ANTIMONY (REFERENCE STATE) Sb	121.750	45.52 0.21	18.178 0.009	0	0	0 107			107
SCANDIUM (REFERENCE STATE) Sc	44.956	34.64 0.21	15.038 0.008	0	0	0 107			107
SELENIUM (REFERENCE STATE) Se	78.960	42.27 0.05	16.42 0.007	0	0	0 30			75
Se $^{2-}$ AQUEOUS ION STD. STATE, $\nu = 1$	78.960				129000 850	-22.600 0.149	262		
SILICON (REFERENCE STATE) Si	28.086	18.81 0.08	12.056 0.002	0	0	0 107			107
SAMARIUM (REFERENCE STATE) Sm	150.400	69.50 2.09	19.98 0.03	0	0	0 107			107
TIN (REFERENCE STATE) Sn	118.690	51.20 0.42	16.289 0.005	0	0	0 107			107
STRONTIUM (REFERENCE STATE) Sr	87.620	55.40 0.17	33.921 0.020	0	0	0 124			107
Sr $^{2+}$ AQUEOUS ION STD. STATE, $\nu = 1$	87.620	-33.00 0.85		-545800 120	-559440 120	98.012 0.021	214		214
TANTALUM (REFERENCE STATE) Ta	180.948	41.51 0.17	10.851 0.005	0	0	0 107			107
TERBIUM (REFERENCE STATE) Tb	158.925	73.30 0.84	19.29 0.03	0	0	0 107			107
TELLURIUM (REFERENCE STATE) Te	127.600	49.50 0.42	20.476 0.008	0	0	0 107			107

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume $v_m^0$ cm <sup>3</sup>	$\Delta H_f^0$ , 298 J/mol	$\Delta G_f^0$ , 298 J/mol	log $K_f$	References $\Delta H_f^0$ S $\Delta G_f^0$ C P
ELEMENTS							
THORIUM (REFERENCE STATE) Th	232.038	53.39 0.84	19.788 0.010	0	0	0 107	107
TITANIUM (REFERENCE STATE) Ti	47.900	30.63 0.08	10.631 0.010	0	0	0 107	107
THALLIUM (REFERENCE STATE) Tl	204.370	64.18 0.21	17.21 0.02	0	0	0 107	107
THULIUM (REFERENCE STATE) Tm	168.934	74.01 0.00	18.126 0.005	0	0	0 107	107
URANIUM (REFERENCE STATE) U	238.029	50.29 0.13	12.497 0.020	0	0	0 107	107
U <sup>+++</sup> AQUEOUS ION STD. STATE, $m = 1$	238.029	-126.00 1.00		-514600 200	-520500 200	91.190 0.035	94 94
U <sup>++++</sup> AQUEOUS ION STD. STATE, $m = 1$	238.029	-326.00 1.00		-613800 200	-579100 200	101.456 0.035	94 94
VANADIUM (REFERENCE STATE) V	50.941	28.91 0.42	8.350 0.004	0	0	0 107	107
TUNGSTEN (REFERENCE STATE) W	183.850	32.64 0.42	9.545 0.004	0	0	0 107	107
YENON (REFERENCE STATE) Xe (IDEAL GAS)	131.300	169.68 0.02	24789.2 3.4	0	0	0 107	107
YTRIUM (REFERENCE STATE) Y	88.906	44.43 0.25	15.038 0.007	0	0	0 107	107
YTERBIUM (REFERENCE STATE) Yb	173.040	59.83 0.17	24.83 0.01	0	0	0 107	107
ZINC (REFERENCE STATE) Zn	65.380	41.63 0.13	9.162 0.007	0	0	0 107	107
Zn <sup>++</sup> AQUEOUS ION STD. STATE, $m = 1$	65.380	-109.60 0.70		-153390 200	-147260 220	25.800 0.039	35 35
ZIRCONIUM (REFERENCE STATE) Zr	91.220	38.99 0.17	14.016 0.007	0	0	0 107	107
METHANE (IDEAL GAS) CH <sub>4</sub>	16.043	186.26 0.21	24789.2 3.4	-74810 335	-50708 377	8.884 0.066	262 262 247
COHENITE Fe <sub>3</sub> C	179.552	104.43 3.35	23.23 0.01	24937 1339	19912 1715	-3.489 0.300	108 108 115
AMMONIA (IDEAL GAS) NH <sub>3</sub>	17.030	192.78 0.08	24789.2 3.4	-45940 350	-16410 350	2.475 0.061	247 215 247
NH <sub>3</sub> UN-IONIZED STD. STATE, $m = 1$	17.031	111.00 0.85		-80290 120	-26600 120	4.660 0.021	262 262
NH <sub>4</sub> <sup>+</sup> AQUEOUS ION STD. STATE, $m = 1$	18.039	111.17 0.75		-133260 250	-79457 301	13.921 0.053	35 35
SULFIDES, ARSENIDES, TELLURIDES, SELENIDES, AND SULFOSALTS							
ACANTHITE (ARGENTITE) Ag <sub>2</sub> S	247.796	142.84 0.42	34.19 0.04	-32346 879	-40080 837	7.022 0.147	80 73 115
REALGAR AsS	106.982	63.51 0.63	29.8 0.24	-71340 2090	-70320 2100	12.320 0.368	274 262
ORPIHENT As <sub>2</sub> S <sub>3</sub>	246.023	163.60 0.40	70.51 0.25	-169030 4200	-168410 4220	29.505 0.739	262 262
BISMUTHINITE Bi <sub>2</sub> S <sub>3</sub>	514.141	200.40 3.30	75.52 0.04	-143090 1050	-140560 1070	24.626 0.187	230 262
OLDHAMITE CaS	72.140	56.65 1.25	27.72 0.09	-474880 2100	-469850 2100	42.316 0.368	120 32 32
GREENOCKITE CdS	144.460	70.29 1.67	29.934 0.015	-149600 1255	-145630 1381	25.514 0.242	120 2 65

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log K <sub>f</sub>	References S $\Delta H_{f,298}^0$ $\Delta G_{f,298}^0$ C <sub>p</sub>
<b>SULFIDES, ARSENIIDES, TELLURIDES, SELENIIDES, AND SULFOSALTS</b>							
COVELLITE CuS	95.606	66.65 1.67	20.42 0.02	-48575 4184	-49080 4226	8.599 0.740	120 65 114
CHALCOCITE Cu <sub>2</sub> S	159.152	120.75 2.09	27.475 0.016	-80115 1255	-86868 1423	15.219 0.249	120 26 115 266 219
CHALCOPYRITE CuFeS <sub>2</sub>	183.513						209
BORNITE Cu <sub>5</sub> FeS <sub>4</sub>	501.817						209
TROILITE FeS	87.907	60.33 0.17	18.2 0.03	-100960 1464	-101333 1506	17.753 0.264	82 220 39 2
PYRRHOTITE Fe <sub>1-8775</sub> S	81.038	60.79 0.21	17.58 0.03				82
PYRITE FeS <sub>2</sub>	119.967	52.93 0.13	23.94 0.007	-171544 1674	-160229 1715	28.072 0.300	80 255 39
MARCASITE FeS <sub>2</sub>	119.967	53.89 0.11	24.58 0.02	-169450 2090	-158421 2090	27.755 0.366	81 81 81
FERROSELITE FeSe <sub>2</sub>	213.767	86.86 0.25	29.96 0.05				80
FRONBERGITE FeTe <sub>2</sub>	311.047	100.20 0.20	38.43 0.05				280
HYDROGEN SULFIDE (IDEAL GAS) H <sub>2</sub> S	34.076	205.80 0.21	24789.2 3.4	-20627 628	-33543 669	5.877 0.117	262 262 247
HS <sup>-</sup> AQUEOUS ION STD. STATE, $\mu = 1$	33.070	62.80 0.85		-16999 850	12100 850	-2.120 0.149	262 262
CINNABAR HgS	232.650	82.51 2.09	28.416 0.015	-58155 2092	-50645 2218	8.873 0.389	137 114 65
METACINNABAR HgS	232.650	96.23 4.18	30.169 0.016	-46735 1506	-43315 837	7.589 0.147	120 72
ALABANDITE RnS	86.998	78.20 1.67	21.46 0.01	-213865 837	-218155 1004	38.220 0.176	120 2 39 49
HAUERITE RnS <sub>2</sub>	119.058	99.91 0.10	34.20 0.01				282
MOLYBDENITE MoS <sub>2</sub>	160.060	62.57 0.21	32.02 0.02	-275300 5000	-266454 5000	46.682 0.880	165 286 61
MILLERITE NiS	90.760	66.11 4.18	16.89 0.01	-84868 4184	-86192 4393	15.101 0.770	80 231 115 274
HEAZLEWOODITE Ni <sub>3</sub> S <sub>2</sub>	240.220	133.90 0.90	40.95 0.02	-202920 1000	-197070 1020	34.526 0.179	274 262
GALENA PbS	239.260	91.38 1.25	31.49 0.01	-97709 962	-96075 837	16.832 0.147	120 245 115 144
CLAUSTHALITE PbSe	286.160	102.51 2.09	34.61 0.01	-102925 2218	-101577 2092	17.796 0.367	120 262
ALTAITE PbTe	334.800	110.04 2.09	40.60 0.01	-70710 1425	-69360 1255	12.152 0.220	120 262
COOPERITE PbS	227.150	55.06 0.13	22.15 0.01	-82425 3350	-76948 3390	13.481 0.594	80 80
STIBNITE Sb <sub>2</sub> S <sub>3</sub>	339.680	182.00 3.30	73.41 0.04	-174890 4180	-173470 4200	30.391 0.736	138 262
HERZBERGITE SbS	150.750	76.82 0.84	29.01 0.02	-106541 1464	-104698 1506	18.343 0.264	120 220 192
STÄNNIC SULFIDE SnS <sub>2</sub>	182.810	87.45 0.18	40.96 0.02				120 192
TUNGSTENITE WS <sub>2</sub>	247.970	94.98 8.37	32.07 0.02	-298320 840	-297945 2680	52.199 0.469	80 65
SPHALERITE ZnS	97.440	58.66 0.84	23.83 0.01	-206900 1700	-202496 1780	35.476 0.312	248 217 208 262

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume $V_m$ cm <sup>3</sup>	$\Delta H_f^0$ , 298 J/mol	$\Delta G_f^0$ , 298 J/mol	Log $K_f$	References $\Delta H_f^0$ S $\Delta G_f^0$ $C_p$
SULFIDES, ARSENIIDES, TELLURIDES, SELENIIDES, AND SULFOSALTS							
WURTZITE ZnS	97.440	58.84 0.12	23.846 0.013	-194570 1520	-190220 1520	33.326 0.266	248 215 208 2
OXIDES AND HYDROXIDES							
CORUNDUM Al <sub>2</sub> O <sub>3</sub>	101.962	50.92 0.10	25.575 0.007	-1675700 1300	-1582228 1320	277.201 0.231	50 35 285 66 159 50
ALUMINUM OXIDE (GAMMA) Al <sub>2</sub> O <sub>3</sub>	101.962	59.83 6.28		-1653517 1260	-1562702 1300	273.780 0.228	32 32 32
BOEHMITE Al(OH) <sub>3</sub>	59.989	48.45 0.21	19.535 0.026	-993054 2110	-918400 2090	160.900 0.366	120 94 115 216
DIASPORE Al(OH) <sub>3</sub>	59.989	35.27 0.17	17.76 0.026	-1000585 5000	-922000 5000	161.530 0.513	120 94 135 216
GIBBSITE Al(OH) <sub>3</sub>	78.004	68.44 0.14	31.956 0.015	-1293128 1192	-1154889 1213	202.333 0.213	95 93 95
ARSENOLITE As <sub>2</sub> O <sub>3</sub>	197.841	107.41 0.13	51.118 0.069	-656970 1674	-575964 1883	100.907 0.330	29 262
CLAUDETITE As <sub>2</sub> O <sub>3</sub>	197.841	113.33 0.13	47.26 0.03	-654795 1715	-575554 1046	100.835 0.183	29 262
BORIC OXIDE B <sub>2</sub> O <sub>3</sub>	69.618	53.97 0.03	27.22 0.06	-1273500 1400	-1194325 1715	209.242 0.300	35 35 247 262
BARUM OXIDE BaO	153.339	72.07 0.38	25.59 0.01	-548100 2090	-520394 2100	91.171 0.368	33 33 33 58 155
BROMELLITE BeO	25.012	13.77 0.04	8.309 0.03	-609400 2500	-580078 2500	101.628 0.438	215 215 32 261
BERYLLIUM OXIDE (BETA) BeO	25.012	16.54 0.03		-601785 3500	-573289 3500	100.438 0.613	32 32 32
BISMITE Bi <sub>2</sub> O <sub>3</sub>	465.959	151.46 2.09	49.73 0.06	-573877 1255	-493453 1464	86.451 0.256	262 262 115 161
CARBON MONOXIDE CO (IDEAL GAS)	28.010	197.67 0.03	24789.2 3.4	-110530 170	-137171 170	24.032 0.030	215 215 247
CARBON DIOXIDE CO <sub>2</sub> (IDEAL GAS)	44.010	213.79 0.04	24789.2 3.4	-393510 130	-394375 167	69.093 0.029	215 215 247 96
CO <sub>3</sub> <sup>=</sup> AQUEOUS ION STD. STATE, m = 1	60.009	-56.90 0.85		-677140 120	-527900 120	92.486 0.021	262 262
HCO <sub>3</sub> <sup>=</sup> AQUEOUS ION STD. STATE, m = 1	61.017	91.20 0.85		-691990 120	-586850 120	102.814 0.021	262 262
H <sub>2</sub> CO <sub>3</sub> UN-IONIZED STD. STATE, m = 1	62.025	187.00 0.85		-699650 120	-623170 120	109.177 0.021	262 262
CALCIUM OXIDE CaO	56.079	38.21 0.13	16.764 0.005	-635089 879	-603487 900	105.729 0.158	33 33 33
PORTLANDITE Ca(OH) <sub>2</sub>	74.095	83.39 0.42	33.056 0.016	-986085 1255	-898408 1300	157.398 0.228	32 32 32 86 86
MONTEPONITE CdO	128.399	54.81 1.25	15.585 0.010	-258200 837	-228515 920	40.035 0.161	120 262 158
CERIANITE CeO <sub>2</sub>	172.119	62.30 0.08	23.853 0.026	-1088680 1464	-1025380 2929	179.643 0.513	279 235 130 8
CERIUM SESQUIOXIDE (HEXAGONAL, α) Ce <sub>2</sub> O <sub>3</sub>	328.238	150.62 4.18	47.75 0.05	-1796200 8400	-1707940 8400	299.225 1.472	113 235 202 105
CERIUM SESQUIOXIDE (HEXAGONAL, β) Ce <sub>2</sub> O <sub>3</sub>	328.238						202
COBALTOUS OXIDE CoO	74.933	52.97 0.34	11.64 0.02	-237940 1255	-214194 1297	37.526 0.227	120 263 129
ESKOLAITE Cr <sub>2</sub> O <sub>3</sub>	151.990	81.17 1.25	29.09 0.032	-1134700 8370	-1053056 8400	184.492 1.472	33 33 33 158



Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References $\Delta H_{f,298}^0$ S $\Delta G_{f,298}^0$ C P
OXIDES AND HYDROXIDES							
DICESIUM MONOXIDE Cs <sub>2</sub> O	281.810	146.87 0.44	59.62 0.07	-345975 1170	-308360 1190	54.023 0.208	59 236 59
CAESIUM HYDROXIDE CsOH	149.911	98.74 4.18		-416726 837	-370690 850	64.944 0.149	32 32 32
TEMORITE CuO	79.545	42.63 0.21	12.22 0.03	-157320 1255	-129564 1297	22.699 0.227	120 263 164 164
CUPRITE Cu <sub>2</sub> O	143.091	93.14 1.67	23.437 0.016	-168610 6276	-146030 6318	25.584 1.107	263 263 164 164
DYSPROSIUM SESQUIOXIDE (CUBIC) Dy <sub>2</sub> O <sub>3</sub>	372.998	149.79 0.85	45.683 0.010	-1863130 3930	-1771385 4000	310.341 0.701	235 235 202 103
ERBIUM SESQUIOXIDE (CUBIC) Er <sub>2</sub> O <sub>3</sub>	382.518	155.64 0.85	44.171 0.010	-1897860 1920	-1808879 2000	316.909 0.350	235 235 207 247
EUROPIUM OXIDE EuO	167.959	62.76 0.85	20.475 0.008	-592040 8370	-556082 8370	97.424 1.466	235 235 166
EUROPIUM SESQUIOXIDE (MONOCLINIC) Eu <sub>2</sub> O <sub>3</sub>	351.918	146.44 8.50	44.02 0.05	-1651420 8400	-1555158 8400	272.458 1.472	281 235 210 57
EUROPIUM SESQUIOXIDE (CUBIC) Eu <sub>2</sub> O <sub>3</sub>	351.918		48.29 0.03				210
MUSTITE Fe <sub>4</sub> O	68.887	57.59 0.42	12.04 0.04	-266270 837	-245155 879	42.950 0.154	120 109 44 247 247
FEROUS OXIDE (STOICHIOMETRIC) FeO	71.846	59.80 1.67	12.00 0.05	-272043 2092	-251156 2176	44.001 0.381	247 247 247
HEMATITE Fe <sub>2</sub> O <sub>3</sub>	159.692	87.40 0.21	30.274 0.012	-824640 1255	-742683 1297	130.267 0.227	78 46 44 247 84 78
MAGNETITE Fe <sub>3</sub> O <sub>4</sub>	231.539	146.14 0.42	44.524 0.008	-1115726 2092	-1012566 2134	177.398 0.374	79 84 44 247 79
GOTHITE FeO(OH)	88.854	60.38 0.63	20.82 0.04	-559330 730	-488550 750	85.591 1.39	139 13
GALLIUM SESQUIOXIDE Ga <sub>2</sub> O <sub>3</sub>	187.438	84.98 0.42	28.941 0.006	-1089100 850	-998342 850	174.906 0.149	120 262 203 145
GADOLINIUM SESQUIOXIDE (MONOCLINIC) Gd <sub>2</sub> O <sub>3</sub>	362.498	151.88 0.85	43.4 0.04	-1819620 3600	-1732338 3600	303.500 0.631	281 235 210
GADOLINIUM SESQUIOXIDE (CUBIC) Gd <sub>2</sub> O <sub>3</sub>	362.498		47.585 0.008				210
GERMANIUM DIOXIDE (QUARTZ TYPE) GeO <sub>2</sub>	104.589	55.27 0.27	24.44 0.04	-551030 800	-497074 900	87.086 0.158	120 262 119 83 5
GERMANIUM DIOXIDE GLASS GeO <sub>2</sub>	104.589	64.50 0.30	28.6 0.1	-526350 630	-475180 710	83.250 0.124	163 119
WATER H <sub>2</sub> O (LIQUID)	18.015	69.95 0.08	18.069 0.003	-285830 42	-237141 84	41.546 0.015	35 35 247 196
OH <sup>-</sup> AQUEOUS ION STD. STATE, $\mu = 1$	17.007	-10.71 0.20		-230025 45	-157328 90	27.563 0.016	35 35
STEAM H <sub>2</sub> O (IDEAL GAS)	18.015	188.72 0.04	24789.2 3.4	-241814 42	-228569 84	40.044 0.015	35 35 247 196
HAFNIUM DIOXIDE HfO <sub>2</sub>	210.489	59.33 0.42	20.823 0.008	-1144740 1255	-1088276 1297	190.662 0.227	120 264 188
HOWTBOIDITE HfO	216.589	70.27 0.34	19.32 0.02	-90789 50	-58528 60	10.254 0.011	247 247 247 258
HOLMIUM SESQUIOXIDE (CUBIC) Ho <sub>2</sub> O <sub>3</sub>	377.859	158.16 0.32	44.90 0.02	-1880700 4850	-1791373 5000	313.842 0.876	235 235 207
DIPOTASSIUM MONOXIDE K <sub>2</sub> O	94.195	94.14 6.28	40.38 0.20	-363171 2092	-322087 2845	56.429 0.498	247 247 247
POTASSIUM SUPEROXIDE KO <sub>2</sub>	71.097	122.50 4.18	32.84 0.04	-284512 2092	-240586 2800	42.150 0.491	32 32 32
POTASSIUM HYDROXIDE KOH	56.105	78.91 0.84	27.45 0.02	-424676 418	-378932 500	66.388 0.088	32 32 32

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume $V_m$ $\text{cm}^3$	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References S ΔG <sub>f</sub> <sup>0</sup> C <sub>p</sub> <sup>0</sup>
OXIDES AND HYDROXIDES							
LANTHANUM SESQUIOXIDE $\text{La}_2\text{O}_3$	325.809	127.32 0.84	49.56 0.02	-1793680 1590	-1705963 1600	298.879 0.280	235 235 142
LITHIUM MONOXIDE $\text{Li}_2\text{O}$	29.879	37.57 0.08	14.76 0.01	-598730 2092	-561985 2134	98.458 0.374	247 247 247
LITHIUM HYDROXIDE $\text{LiOH}$	23.947	42.80 0.21	16.44 0.05	-484926 159	-438941 159	76.901 0.028	215 215 32
LUTETIUM SESQUIOXIDE (CUBIC) $\text{Lu}_2\text{O}_3$	397.938	109.96 0.85	42.22 0.01	-1878200 7530	-1788849 6280	313.400 1.100	281 235 202
PERICLASE $\text{MgO}$	40.304	26.94 0.17	11.248 0.004	-601490 290	-569196 300	99.721 0.053	215 215 261 247 204
BRUCITE $\text{Mg}(\text{OH})_2$	58.320	63.18 0.13	24.63 0.07	-924540 440	-833506 440	146.027 0.077	214 214 131 102
MANGANOSITE $\text{MnO}$	70.937	59.71 0.42	13.221 0.004	-385220 460	-362896 502	63.578 0.088	120 263 242
PYROLUSITE $\text{MnO}_2$	86.937	53.05 0.42	16.61 0.02	-520030 837	-465138 879	81.491 0.154	120 263 168
BIXBYITE $\text{Mn}_2\text{O}_3$	157.874	110.46 2.09	31.37 0.05	-958970 2092	-881068 2218	154.360 0.389	120 263 115 197 191
HAUSMANNITE $\text{Mn}_3\text{O}_4$	228.812	153.97 4.18	46.95 0.06	-1387830 1674	-1282774 2092	224.738 0.367	197 263 241 197
MOLYBDENUM DIOXIDE $\text{MoO}_2$	127.939	50.02 0.30	19.58 0.02	-587850 2090	-533053 2510	93.389 0.440	247 247 247 159
MOLYBDITE $\text{MoO}_3$	143.938	77.74 0.42	30.56 0.04	-745170 418	-668055 460	117.041 0.081	247 247 247 159 140
NITROGEN DIOXIDE $\text{NO}_2$ (IDEAL GAS)	46.005	240.06 0.08	24789.2 3.4	33095 418	51251 460	-8.979 0.081	247 247 247
$\text{NO}_3^-$ AQUEOUS ION STD. STATE, $m = 1$	62.005	146.94 0.85		-207400 420	-111500 400	19.534 0.070	35 35
DISODIUM MONOXIDE $\text{Na}_2\text{O}$	61.979	75.27 0.84	25.88 0.08	-414820 280	-376089 290	65.890 0.051	247 183 247 265 63
SODIUM HYDROXIDE $\text{NaOH}$	39.997	64.43 0.84	18.78 0.06	-425800 85	-379651 125	66.514 0.022	32 215 32 32
NIOBIUM MONOXIDE $\text{NbO}$	108.906	46.02 8.40	14.97 0.01	-419660 12550	-391945 12550	68.667 2.199	33 33 33
NIOBIUM DIOXIDE $\text{NbO}_2$	124.905	54.51 0.30	45.02 0.04	-794960 8370	-739194 8370	129.504 1.466	33 33 33 130
DINIIOBIUM PENTOXIDE $\text{Nb}_2\text{O}_5$	265.810	137.32 1.26	93.42 0.10	-1899536 4184	-1765859 4200	309.373 0.736	33 33 189
NEODYMIUM SESQUIOXIDE (HEXAGONAL) $\text{Nd}_2\text{O}_3$	336.478	158.57 4.20	45.92 0.02	-1807910 1000	-1721048 1020	301.522 0.179	235 235 210
BUNSENITE $\text{NiO}$	74.699	37.99 0.17	10.97 0.02	-239743 418	-211581 460	37.068 0.081	120 23 129 263
PHOSPHORUS MONOXIDE $\text{PO}$ (IDEAL GAS)	46.973	222.77 0.02	24789.2 3.4	-12134 4184	-41157 4200	7.211 0.736	32 32 32
PHOSPHORUS PENTOXIDE $\text{P}_2\text{O}_5$	141.945	115.50 0.40	59.4 0.2	-1470000 4200	-1337897 4200	234.396 0.736	215 215 247
PHOSPHORUS PENTOXIDE (DIMERIC) $(\text{P}_2\text{O}_5)_2$	283.889	231.00 0.80	118.8 0.4	-2940000 8400	-2675794 8400	468.791 1.470	215 215 247
$\text{PO}_4^{3-}$ AQUEOUS ION STD. STATE, $m = 1$	94.971	-222.00 4.20		-1259550 850	-1001550 850	175.469 0.149	262 262
ORTHOPHOSPHORIC ACID (CRYSTAL) $\text{H}_3\text{PO}_4$	97.995	110.54 0.42	48.52 0.01	-1266920 2090	-1112290 2510	194.869 0.440	32 32 32
ORTHOPHOSPHORIC ACID (LIQUID) $\text{H}_3\text{PO}_4$	97.995	150.78 4.20		-1254200 2090	-1111700 2510	194.766 0.440	32 32 32
LITHARGE (RED) $\text{PbO}$	223.199	66.32 0.84	23.91 0.05	-219409 830	-189202 900	33.148 0.158	32 32 32

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References $\Delta H_f^0$ S $\Delta G_f^0$ C <sub>P</sub>
OXIDES AND HYDROXIDES							
MASSICOT (YELLOW) PbO	223.199	68.70 0.21	23.15 0.03	-218070 630	-188573 700	33.037 0.123	32 32 32
PLATTNERITE PbO <sub>2</sub>	239.199	71.80 0.42	25.01 0.01	-274470 2929	-215314 3000	37.722 0.526	32 32 32
MINIUM Pb <sub>3</sub> O <sub>4</sub>	686.598	211.96 6.69	76.81 0.09	-718686 6276	-601358 6300	105.356 1.104	32 32 32
PRASEODYMIUM SESQUIOXIDE (HEX) Pr <sub>2</sub> O <sub>3</sub>	329.814	158.57 4.20	46.53 0.05	-1809580 6690	-1721025 6700	301.518 1.174	281 235 200
PRASEODYMIUM OXIDE PrO <sub>1.833</sub>	170.235	79.91 4.20	24.6 0.2	-1904560 6690	-1796610 6700	314.760 1.174	281 281 200
RHENIUM DIOXIDE (ORTHORHOMBIC) ReO <sub>2</sub>	218.206	47.82 0.05	18.80 0.01	-451870 3350	-394070 3360	69.040 0.589	249 133 249
RHENIUM TRIOXIDE ReO <sub>3</sub>	234.205	69.24 0.09	31.78 0.01	-593710 2930	-511700 2940	89.648 0.515	249 133 249
DIRHENIUM HEPTOXIDE Re <sub>2</sub> O <sub>7</sub>	484.410	207.30 0.40	77.95 0.09	-1274030 6280	-1099980 6290	192.713 1.102	249 133 249
SULFUR DIOXIDE SO <sub>2</sub> (IDEAL GAS)	64.059	248.22 0.06	24789.2 3.4	-296810 200	-300170 251	52.589 0.044	35 35 247
SULFUR TRIOXIDE SO <sub>3</sub> (IDEAL GAS)	80.058	256.76 0.84	24789.2 3.4	-395722 711	-371046 795	65.006 0.139	247 247 247
SO <sub>4</sub> <sup>2-</sup> AQUEOUS ION STD. STATE, n = 1	80.058	-29.00 4.20		-635600 850	-486600 850	85.251 0.149	262 262
SO <sub>4</sub> <sup>2-</sup> AQUEOUS ION STD. STATE, n = 1	96.058	20.00 0.85		-909270 120	-744630 120	130.457 0.021	262 262
VALENTINITE Sb <sub>2</sub> O <sub>3</sub>	291.498	123.01 2.51	50.01 0.05	-708560 2930	-626345 3054	109.733 0.535	262 262
SCANDIUM SESQUIOXIDE Sc <sub>2</sub> O <sub>3</sub>	137.910	76.99 0.42	35.91 0.01	-1908820 2510	-1819371 2520	318.748 0.441	281 264 203
SILICON MONOXIDE SiO (IDEAL GAS)	44.085	211.57 0.84	24789.2 3.4	-100416 8368	-127305 8500	22.304 1.489	247 247 247
QUARTZ SiO <sub>2</sub>	60.085	41.46 0.20	22.688 0.001	-910700 1000	-856288 1100	150.019 0.193	35 35 247
H <sub>4</sub> SiO <sub>4</sub> UN-IONIZED STD. STATE, n = 1	96.115	180.00 4.20		-1460000 1700	-1308000 1700	229.157 0.298	262 171
CRISTOBALITE SiO <sub>2</sub>	60.085	43.40 0.13	25.739 0.033	-908346 2090	-854512 2130	149.704 0.373	247 247 247
TRIDYMITE SiO <sub>2</sub>	60.085	43.93 0.42	26.53 0.20	-907488 2385	-853812 2427	149.585 0.425	285 148 172
COESITE SiO <sub>2</sub>	60.085	40.38 0.42	20.641 0.001	-905584 2092	-850850 2134	149.066 0.374	101 101 285
STISHOVITE SiO <sub>2</sub>	60.085	27.78 0.42	14.014 0.009	-861318 2092	-802827 2134	140.653 0.374	101 101 285
SILICON DIOXIDE GLASS SiO <sub>2</sub>	60.085	47.40 0.21	27.27 0.10	-903200 2092	-850559 2134	149.015 0.374	285 148 52
SAMARIUM SESQUIOXIDE (MONOCLINIC) Sm <sub>2</sub> O <sub>3</sub>	348.798	151.04 4.20	45.04 0.02	-1822970 2010	-1796690 2020	314.774 0.354	235 235 210
SAMARIUM SESQUIOXIDE (CUBIC) Sm <sub>2</sub> O <sub>3</sub>	348.798		49.10 0.01				7 193
CASSITERITE SnO <sub>2</sub>	150.689	52.30 1.25	21.55 0.03	-580740 628	-519902 753	91.085 0.132	120 262 115
STRONTIUM OXIDE SrO	103.619	55.52 0.42	20.686 0.005	-590490 920	-560353 930	98.172 0.163	33 24 33
DITANTALUM PENTOXIDE (BETA) Ta <sub>2</sub> O <sub>5</sub>	441.893	143.13 1.26	53.17 0.05	-2045976 4184	-1910984 4200	334.798 0.736	33 33 33

Name and Formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume $V_m$ cm <sup>3</sup>	$\Delta H_f^0, 298$ J/mol	$\Delta G_f^0, 298$ J/mol	Log $K_f$	References $\Delta H_f^0$ $\Delta G_f^0$ C <sub>P</sub>
OXIDES AND HYDROXIDES							
TERBIUM SESQUIOXIDE (CUBIC) Tb <sub>2</sub> O <sub>3</sub>	365.849	156.90 4.20	46.48 0.02	-1865230 8370	-1776553 8400	311.246 1.472	281 235 200
TERBIUM OXIDE TbO <sub>1.714</sub>	186.348	80.75 4.20		-953950 4180	-938980 4200	164.506 0.736	281 235 200
TERBIUM OXIDE TbO <sub>1.812</sub>	187.916	81.17 4.20		-960230 4180	-942180 4200	165.067 0.736	281 235 200
TELLURITE TeO <sub>2</sub>	159.599	79.50 4.20	27.75 0.02	-322590 850	-270370 850	47.370 0.149	262 262
THORIANITE ThO <sub>2</sub>	264.037	65.23 0.21	26.373 0.007	-1226410 3510	-1168775 3510	204.765 0.615	215 215 260
TITANIUM MONOXIDE TiO	63.899	34.77 2.10	13.00 0.01	-542660 12550	-513312 12550	89.931 2.199	33 33 176
RUTILE TiO <sub>2</sub>	79.899	50.29 0.17	18.82 0.008	-944750 1260	-889446 1030	155.828 0.180	33 33 33 215 176
ANATASE TiO <sub>2</sub>	79.899	49.91 0.29	20.52 0.03	-938720 2090	-883303 2090	154.752 0.366	33 33 176
DITITANIUM TRIOXIDE Ti <sub>2</sub> O <sub>3</sub>	143.798	77.25 0.21	31.43 0.02	-1520884 8368	-1433903 8370	251.215 1.466	33 33 33 176
TRITITANIUM PENTOXIDE (ALPHA) Ti <sub>3</sub> O <sub>5</sub>	223.697	129.37 1.67	52.69 0.03	-2459150 4180	-2317411 4600	406.003 0.806	33 33 176
TETRATITANIUM HEPTOXIDE Ti <sub>4</sub> O <sub>7</sub>	303.596	198.74 12.00		-3404520 6280	-3213166 6280	562.936 1.100	33 33 33
THULIUM SESQUIOXIDE Tm <sub>2</sub> O <sub>3</sub>	385.867	139.75 0.85	43.42 0.01	-1888660 850	-1794446 850	314.381 0.149	235 235 207
URANINITE UO <sub>2</sub>	270.028	77.03 0.24	24.618 0.014	-1084910 1000	-1031770 1000	180.763 0.175	110 41 77 215 215 60
URANIUM TRIOXIDE (GAMMA) UO <sub>3</sub>	286.027	98.62 0.25	35.56 0.04	-1223800 800	-1146461 1000	200.856 0.175	112 215 170 215
VANADIUM MONOXIDE VO	66.941	39.01 0.85	10.26 0.03	-431790 6280	-404219 6280	70.818 1.100	33 33 115 191
KAPILANITE V <sub>2</sub> O <sub>3</sub>	149.881	98.07 1.25	29.85 0.03	-1218800 6280	-1139052 6500	199.558 1.139	33 33 38
DIVANADIUM TETROXIDE V <sub>2</sub> O <sub>4</sub>	165.880	103.52 2.09		-1427162 6276	-1318457 6500	230.989 1.139	33 33 38
DIVANADIUM PENTOXIDE V <sub>2</sub> O <sub>5</sub>	181.880	130.54 2.09	53.94 0.04	-1550590 6276	-1419435 6300	248.680 1.104	33 33 38
TUNGSTEN DIOXIDE WO <sub>2</sub>	215.849	50.53 0.29	19.92 0.03	-589690 880	-533858 960	93.530 0.168	247 247 140
TUNGSTEN TRIOXIDE WO <sub>3</sub>	231.848	75.91 1.26	31.61 0.10	-842909 837	-764062 879	133.861 0.154	247 247 140
YTRBIUM SESQUIOXIDE (CUBIC) Y <sub>2</sub> O <sub>3</sub>	225.810	99.08 4.20	44.88 0.02	-1905310 2260	-1816609 2400	318.264 0.420	264 264 210
YTERBIUM SESQUIOXIDE (CUBIC) Yb <sub>2</sub> O <sub>3</sub>	394.078	133.05 0.85	42.76 0.01	-1814600 850	-1726844 850	302.537 0.149	235 235 207
ZINCITE ZnO	81.379	43.64 0.40	14.338 0.005	-350460 270	-320477 300	56.146 0.053	120 41 115 215 215
BADDELEYITE ZrO <sub>2</sub>	123.219	50.38 0.34	21.15 0.01	-1100560 1674	-1042790 1715	182.693 0.300	264 264 43 104
MULTIPLE OXIDES							
TIALITE Al <sub>2</sub> TiO <sub>5</sub>	181.861	109.62 0.84	48.75 0.05				120 21
CHRYSOBERYL BeAl <sub>2</sub> O <sub>4</sub>	126.974	66.28 0.13	34.32 0.023	-2300780 2800	-21708460 2800	381.659 0.149	214 214 67

Name and formula	Formula weight g	Entropy S <sub>298</sub> J/mol·K	Molar volume cm <sup>3</sup>	ΔH <sub>f,298</sub> <sup>o</sup> J/mol	ΔG <sub>f,298</sub> <sup>o</sup> J/mol	Log K <sub>f</sub>	References S ΔG <sub>f</sub> <sup>o</sup> C <sub>p</sub>
MULTIPLE OXIDES							
CALCIUM FERRITE CaFe <sub>2</sub> O <sub>4</sub>	215.772 0.84	145.35 0.84	44.98 0.05	-1520340 120	-1412666 120	247.494 0.021	214 214 20
DICALCIUM FERRITE Ca <sub>2</sub> Fe <sub>2</sub> O <sub>5</sub>	271.851 1.26	188.78 1.26	67.18 0.10	-2139280 850	-2001560 850	350.667 0.149	214 214 20
PEROVSKITE CaTiO <sub>3</sub>	135.978 0.42	93.64 0.42	33.626 0.01	-1660630 1715	-1575256 1757	275.980 0.308	120 214 177
COBALT SPINEL Co <sub>3</sub> O <sub>4</sub>	240.797 0.84	102.51 0.84	39.77 0.02	-891190 8500	-772553 8500	135.349 1.489	263 263 129
HERCYNITE FeAl <sub>2</sub> O <sub>4</sub>	173.809 0.84	106.27 0.84	40.75 0.05	-1966480 8500	-1850795 8500	324.253 1.489	120 263
CHRONITE FeCr <sub>2</sub> O <sub>4</sub>	223.837 1.67	146.02 1.67	44.01 0.10				120 174
ILMENITE FeTiO <sub>3</sub>	151.745 1.25	105.86 1.25	31.69 0.08	-1236622 1590	-1159170 1632	203.083 0.286	120 122 177
TITANOMAGNETITE Fe <sub>2</sub> TiO <sub>4</sub>	223.592 2.51	168.87 2.51	46.82 0.05				120 21
PSUEDOBROOKITE Fe <sub>2</sub> TiO <sub>5</sub>	239.591 1.25	156.48 1.25	54.53 0.05				120 21
LITHIUM ALUMINATE (ALPHA) LiAlO <sub>2</sub>	65.921 2.10	53.35 2.10	25.21 0.01	-1188670 4180	-1126276 4180	197.320 0.732	32 32 32
SPINEL MgAl <sub>2</sub> O <sub>4</sub>	142.267 0.42	80.63 0.42	39.71 0.03	-2299320 750	-2174860 760	381.028 0.133	214 237 22 31
PICROCHROMITE MgCr <sub>2</sub> O <sub>4</sub>	192.295 0.84	106.02 0.84	43.56 0.05	-1783640 850	-1669079 850	292.417 0.149	214 214 174
MAGNESIOFERRITE MgFe <sub>2</sub> O <sub>4</sub>	199.997 0.84	123.85 0.84	44.57 0.05	-1428420 1841	-1317004 1883	230.735 0.330	120 214 20 146
GEIKELITE MgTiO <sub>3</sub>	120.203 0.42	74.56 0.42	30.86 0.07	-1572765 1130	-1484371 1172	260.057 0.205	120 214 177
TREVORITE NiFe <sub>2</sub> O <sub>4</sub>	234.392 0.84	131.80 0.84	43.65 0.05	-1081150 850	-972940 850	170.456 0.149	120 263
ZINC TITANIUM SPINEL Zn <sub>2</sub> TiO <sub>4</sub>	242.658 0.28	143.09 0.28	45.58 0.02	-1647660 2510	-1534035 2510	268.758 0.440	264 264 21 253
HALIDES							
BROMARGYRITE AgBr	187.772 0.42	107.11 0.42	28.991 0.008	-100580 180	-97121 180	17.015 0.032	120 215 115 215
POTASSIUM BROMIDE KBr	119.002 0.20	95.90 0.20	43.28 0.01	-393460 180	-380061 180	66.585 0.032	215 215 247 173
STRONTIUM BROMIDE SrBr <sub>2</sub>	247.428 0.20	135.10 0.20	58.31 0.06	-717540 850	-695908 850	121.921 0.149	250 214 250
TITANIUM TRIBROMIDE TiBr <sub>3</sub>	287.612 3.35	176.44 3.35	67.8 0.09	-595380 8370	-570732 8450	99.990 1.480	247 247 141
CHLORARGYRITE AgCl	143.321 0.20	96.23 0.20	25.727 0.007	-127070 85	-109819 85	19.240 0.015	120 215 115 215
HYDROPHILITE CaCl <sub>2</sub>	110.986 1.25	104.60 1.25	50.75 0.005	-795800 650	-748063 750	131.058 0.131	214 214 115 169
LAWRENCEITE FeCl <sub>2</sub>	126.753 0.42	117.95 0.42	39.46 0.21	-341650 420	-302172 420	52.940 0.074	215 215 169 147
MOLYSITE FeCl <sub>3</sub>	162.206 0.42	142.26 0.42	57.86 0.10	-399240 420	-333754 1420	58.473 0.249	215 215 169 147
HYDROGEN CHLORIDE HCl (IDEAL GAS)	36.461 0.03	186.90 0.03	24789.2 3.4	-92312 130	-95299 130	16.696 0.023	215 215 247
CALOMEL HgCl	236.043 1.25	96.23 1.25	32.939 0.075	-132610 1255	-105415 1339	18.469 0.235	263 263

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol-K	Molar volume $v_m^0$ cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References S A U C P
HALIDES							
SYLVITE KCl	74.551	82.59 0.20	37.524 0.004	-436470 140	-408554 140	71.577 0.025	215 215 247 173
CHLOROMAGNESITE MgCl <sub>2</sub>	95.211	89.62 0.84	40.81 0.10	-641320 460	-591785 544	103.679 0.095	120 214 169 247 247
SCACCHITE MnCl <sub>2</sub>	125.844	118.24 0.21	42.11 0.17	-481290 837	-440488 879	77.172 0.154	34 214 169 147
SALAMMONIAC NH <sub>4</sub> Cl	53.491	95.02 0.40	35.06 0.05	-315190 290	-203776 290	35.701 0.051	215 215 247 215 247
HALITE NaCl	58.443	72.12 0.21	27.015 0.003	-411260 110	-384212 110	67.313 0.019	215 215 247 215 247
WICKEL CHLORIDE NiCl <sub>2</sub>	129.606	97.66 0.21	36.7 0.07	-305330 80	-259030 80	45.381 0.014	263 263 40 263 263
COTUNNITE PbCl <sub>2</sub>	278.106	135.98 2.09	47.09 0.05	-359400 293	-314033 711	55.018 0.125	120 247 115 215 215
TITANIUM TRICHLORIDE TiCl <sub>3</sub>	154.259	139.75 1.26	57.3 0.3	-721740 4180	-654507 5020	114.667 0.879	247 247 141 247 247
URANIUM TRICHLORIDE UCl <sub>3</sub>	344.388	158.95 0.40	62.04 0.06	-891190 4000	-823820 5000	144.330 0.876	70 89 70 233
URANIUM TETRACHLORIDE UCl <sub>4</sub>	379.841	196.60 0.50	77.6 0.03	-1018390 3000	-928850 3000	162.731 0.526	70 89 70 233
VANADIUM DICHLORIDE VCl <sub>2</sub>	121.847	97.07 1.26	35.06 0.05	-451870 8500	-405641 8500	71.074 1.489	120 264 125 120 264
VANADIUM TRICHLORIDE VCl <sub>3</sub>	157.300	130.96 1.70	54.48 0.1	-580740 850	-511399 850	89.595 0.149	120 264 125 120 264
ALUMINUM TRIFLUORIDE AlF <sub>3</sub>	83.977	66.48 0.42	26.15 0.1	-1510400 1300	-1431076 1300	250.720 0.228	247 247 51 215 215 181
FLUORITE CaF <sub>2</sub>	78.077	68.87 0.34	24.542 0.007	-1229260 420	-1176920 420	206.192 0.074	120 215 175 120 215
HYDROGEN FLUORIDE HF (IDEAL GAS)	20.006	173.78 0.04	24789.2 3.4	-273300 700	-275400 700	48.249 0.123	35 35 247 35 35
SELLAITE MgF <sub>2</sub>	62.302	57.25 0.42	19.61 0.01	-1124200 1200	-1071064 1200	187.647 0.210	247 215 175 247 215
VILLIAUMITE NaF	41.988	51.30 0.08	14.984 0.005	-576550 670	-546319 670	95.713 0.117	215 215 181 215 215
CRYOLITE Na <sub>3</sub> AlF <sub>6</sub>	209.942	238.45 1.67	70.81 0.20	-3309544 4180	-3144915 4300	550.978 0.753	247 247 181 247 247
URANIUM TETRAFLUORIDE UF <sub>6</sub>	314.023	151.67 0.17	46.88 0.08	-1853500 5000	-1762800 5100	308.837 0.894	70 233 70 233 233
IODARGYRITE AgI	234.772	115.48 1.67	41.301 0.04	-61840 1674	-66254 1757	11.607 0.308	120 263 115 263 263
COCCINITE HgI <sub>2</sub>	454.399	181.33 6.28	71.84 0.10	-105437 1674	-102203 2552	17.906 0.447	263 263 115 32 247 32
CARBONATES AND NITRATES							
WITHERITE BaCO <sub>3</sub>	197.349	112.13 2.09	45.81 0.06	-1210850 2230	-1132210 2240	198.359 0.392	120 4 155 120 4
ARAGONITE CaCO <sub>3</sub>	100.089	87.99 0.20	34.15 0.05	-1207430 1423	-1127793 1464	197.586 0.256	243 214 115 243 214
CALCITE CaCO <sub>3</sub>	100.089	91.71 0.20	36.934 0.015	-1207370 1339	-1128842 1381	197.769 0.242	243 214 115 243 214
VATERITE CaCO <sub>3</sub>	100.089		37.63 0.07		-1125540 1500	197.191 0.263	256 256
MONOHYDROCALCITE CaCO <sub>3</sub> ·H <sub>2</sub> O	118.104		48.7 0.4	-1498290 1170	-1361600 1130	238.548 0.198	106 106
DOLOMITE CaMg(CO <sub>3</sub> ) <sub>2</sub>	184.403	155.18 0.29	64.34 0.03	-2324480 1460	-2161672 1670	378.718 0.293	244 225 151 244 225

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References $\Delta H_f^0$ S $\Delta G_f^0$ C <sup>p</sup>
CARBONATES AND NITRATES							
HUMITE CaHg <sub>2</sub> (CO <sub>3</sub> ) <sub>4</sub>	353.032	299.53 0.88	122.58 0.10	-4529600 1570	-4203425 1630	736.426 0.286	91 92
OTAVITE CdCO <sub>3</sub>	172.409	92.47 2.51	34.3 0.02	-750610 2510	-669440 2636	117.284 0.462	120 262
MALACHITE Cu <sub>2</sub> (CO <sub>3</sub> )(OH) <sub>2</sub>	221.116		54.86 0.08	-1053950 2090			218
AZURITE Cu <sub>3</sub> (OH) <sub>2</sub> (CO <sub>3</sub> ) <sub>2</sub>	344.671		91.01 0.13	-1632180 2000			263
SIDERITE FeCO <sub>3</sub>	115.856	105.0 2.5	29.378 0.014	-736985 2259	-666698 2092	116.803 0.367	220 263 117
MAGNESITE HgCO <sub>3</sub>	84.314	65.09 0.14	28.018 0.013	-1113280 1339	-1029480 1381	180.360 0.242	95 220 115
MESQUEHONITE HgCO <sub>3</sub> ·3H <sub>2</sub> O	138.360	195.62 0.59	75.47 0.05	-1977260 260	-1723746 500 <sup>a</sup>	301.994 0.088	223 224
HYDROMAGNESITE 5HgO·4CO <sub>2</sub> ·5H <sub>2</sub> O	467.637	503.67 1.55	211.1 0.1	-6514860 1060	-5864166 1090	1027.382 0.191	223 224
ARTINIITE Hg <sub>2</sub> (OH) <sub>2</sub> CO <sub>3</sub> ·3H <sub>2</sub> O	196.679	232.92 0.67	96.43 0.10	-2920610 710	-2568346 750	449.966 0.131	91 92
RHODOCHROSITE MnCO <sub>3</sub>	114.947	100.0 2.1	31.073 0.014	-889270 1213	-816047 1381	142.968 0.242	220 220 168 68
DAWSONITE NaAlCO <sub>3</sub> (OH) <sub>2</sub>	143.996	132.00 0.50	59.3 0.3	-1963970 2930	-1785990 2950	312.900 0.517	55 55 55
CERUSSITE PbCO <sub>3</sub>	267.209	130.96 3.35	40.59 0.06	-699150 1172	-625337 1548	109.557 0.271	120 214 4
STROMIANTITE SrCO <sub>3</sub>	147.629	97.07 1.67	39.01 0.06	-1218680 1450	-1137640 1460	199.311 0.256	120 4 155
SMITHSONITE ZnCO <sub>3</sub>	125.389	82.42 1.25	28.275 0.013	-812780 2930	-731480 2970	128.153 0.521	120 214
NITROBARITE Ba(NO <sub>3</sub> ) <sub>2</sub>	261.350	213.80 0.84	80.58 0.08	-992070 2100	-796579 2500	139.558 0.438	214 214 238
CALCIUM NITRATE Ca(NO <sub>3</sub> ) <sub>2</sub>	164.090	193.30 0.40	66.09 0.03	-938390 1510	-742985 1760	130.168 0.308	214 214 238
NITER KNO <sub>3</sub>	101.103	133.09 0.67	48.04 0.06	-494460 420	-394544 420	69.123 0.074	120 215 115 215
MAGNESIUM NITRATE Mg(NO <sub>3</sub> ) <sub>2</sub>	148.315	164.01 1.60	62.93 0.03	-790650 1300	-589181 1420	103.223 0.249	214 214 238
AMMONIA-NITER NH <sub>4</sub> NO <sub>3</sub>	80.043	151.08 0.21	46.49 0.10	-365560 837	-183803 879	32.202 0.154	262 262 115
SODA-NITER NaNO <sub>3</sub>	84.995	116.52 0.68	37.6 0.02	-468020 420	-367153 420	64.324 0.074	120 215 115 215
STROMIUM NITRATE Sr(NO <sub>3</sub> ) <sub>2</sub>	211.630	194.56 0.50	70.93 0.04	-978220 1000	-779086 1300	136.493 0.228	214 214 250
SULFATES AND BORATES							
ALUMINUM SULFATE Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	396.182	239.32 1.20		-3440840 1800	-3099852 1880	543.084 0.329	262 262 239
BARITE BaSO <sub>4</sub>	233.398	132.21 0.84	52.1 0.06	-1473190 1000	-1362186 1300	238.650 0.228	120 214 115
ANHYDRITE CaSO <sub>4</sub>	136.138	106.69 1.67	45.94 0.06	-1434110 4226	-1321696 4184	231.557 0.733	120 214 115 214
GYPSUM CaSO <sub>4</sub> ·2H <sub>2</sub> O	172.168	194.14 1.25	74.69 0.22	-2022628 4644	-1797197 4602	314.863 0.806	214 214
CHALCOCYANITE CuSO <sub>4</sub>	159.604	109.50 0.60	40.88 0.03	-771360 1300	-662310 1400	116.034 0.245	54 3 54 271 263

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume $v_m$ cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References S $\Delta H_f^0$ $\Delta G_f^0$ $C_p$
SULFATES AND BORATES							
CHALCANTHITE CuSO <sub>4</sub> ·5H <sub>2</sub> O	249.680 4.18	300.41	108.97 0.22	-2279650 3347	-1879796 3598	329.334 0.630	263 263
BROCHANTITE Cu <sub>2</sub> SO <sub>4</sub> (OH) <sub>6</sub>	452.285		113.6 0.2		-1817950 2510	318.499 0.440	263 17
FERRIC SULFATE Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	453.912	282.84 0.85	130.77 0.15	-2576930 2930	-2249555 3010	394.114 0.527	212 14 212
SZOMOLNOKITE FeSO <sub>4</sub> ·H <sub>2</sub> O	169.920		55.9 0.4	-1243900 500			1
MELANTERITE FeSO <sub>4</sub> ·7H <sub>2</sub> O	278.011	409.20 1.30	146.5 0.3	-3014400 600	-2509641 1300	439.681 0.228	120 1
SULFURIC ACID (LIQUID) H <sub>2</sub> SO <sub>4</sub>	98.073	156.90 0.21	53.57 0.07	-813990 418	-689995 460	120.885 0.081	69 262 262 74
ARCANITE K <sub>2</sub> SO <sub>4</sub>	174.254	175.56 0.35	65.5 0.07	-1437700 540	-1319662 540	231.200 0.095	215 215 239
POTASSIUM ALUMINUM SULFATE KAl(SO <sub>4</sub> ) <sub>2</sub>	294.226	204.60 1.26	92.33 0.08	-2470150 1300	-2239790 1380	392.404 0.242	265 265 265
ALUNITE K <sub>2</sub> Al <sub>2</sub> (OH) <sub>12</sub> (SO <sub>4</sub> ) <sub>6</sub>	900.467	656.05 3.77	293.6 0.4				120 121
EPSOMITE MgSO <sub>4</sub> ·7H <sub>2</sub> O	246.469	372.00 4.00	146.8 0.2	-3388700 120	-2871240 850	503.032 0.149	214 214
MANGANESE SULFATE MnSO <sub>4</sub>	150.996	112.13 0.85	43.62 0.04	-1065250 1050	-957326 1300	167.720 0.228	263 263 242
MASCAGHITE (Mn <sub>2</sub> ) <sub>2</sub> SO <sub>4</sub>	132.134	220.08 1.25	74.68 0.09	-1180850 1255	-901677 1339	157.971 0.235	120 262 121 262 239
AMMONIUM BISULFATE NH <sub>4</sub> HSO <sub>4</sub>	115.104		65.07 0.08				239
THENARDITE Na <sub>2</sub> SO <sub>4</sub>	142.037	149.58 0.08	53.33 0.06	-1387790 420	-1269985 420	222.497 0.074	215 215 42
MIRABILITE Na <sub>2</sub> SO <sub>4</sub> ·10H <sub>2</sub> O	322.189	591.90 0.60	219.8 0.4	-4327250 3970	-3646540 3350	638.861 0.587	25 265
RETSCHERSITE (ALPHA, GREEN) NiSO <sub>4</sub> ·6H <sub>2</sub> O	262.849	334.50 0.40	126.6 0.2	-2682800 120	-2224542 120	389.732 0.021	263 263
MORENOSITE NiSO <sub>4</sub> ·7H <sub>2</sub> O	280.864	378.90 0.40	143.8 0.5	-2976300 120	-2461735 120	431.288 0.021	263 263
ANGLESITE PbSO <sub>4</sub>	303.258	148.57 0.29	47.95 0.06	-919940 1088	-813026 1046	142.439 0.183	262 262 115
CELESTITE SrSO <sub>4</sub>	183.678	118.00 4.20	46.25 0.06	-1453170 4200	-1340970 4000	234.933 0.701	120 214 114
ZINKOSITE ZnSO <sub>4</sub>	161.438	110.46 1.25	41.57 0.07	-982820 837	-871530 962	152.689 0.169	271 262 115 3
BIANCHITE ZnSO <sub>4</sub> ·6H <sub>2</sub> O	269.529	363.60 1.30	130.2 0.5	-2777460 120	-2324372 120	407.222 0.021	262 262
GOSLARITE ZnSO <sub>4</sub> ·7H <sub>2</sub> O	287.544	388.70 1.30	145.8 0.1	-3077800 120	-2562652 120	448.968 0.021	262 262
BORAI Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> ·10H <sub>2</sub> O	381.367		222.7 0.2	-6278900 8500			265
PHOSPHATES, MOLYBDATES, CHROMATES, URANATES, AND TUNGSTATES							
BERLINITE AlPO <sub>4</sub>	121.953	90.79 0.21	46.58 0.10	-1716400 2092	-1605875 2134	281.344 0.374	262 262 151
WHITLOCKITE Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	346.213	235.98 0.84	97.62 0.09	-4085925 2100	-3860760 2200	676.394 0.385	214 214 115
HYDROXYAPATITE Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> OH	556.367	390.37 1.67	159.6 0.2	-6669259 5000	-6286093 5000	1101.302 0.876	120 214 52 150



Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume cm <sup>3</sup>	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References S $\Delta H_f^0$ $\Delta G_f^0$ C <sub>p</sub>
<b>PHOSPHATES, MOLYBDATES, CHROMATES, URANATES, AND TUNGSTATES</b>							
FLUORAPATITE Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> F	558.358	387.86 1.67	157.56 0.12	-6819860 5000	-6455778 5000	1131.033 0.876	120 214 52
STRENGITE FePO <sub>4</sub> ·2H <sub>2</sub> O	204.864	171.25 1.25	64.54 0.30	-1870790 854	-1645483 850	288.284 0.149	53 263 53
POWELLITE CaMoO <sub>4</sub>	200.018	122.59 0.84	47.0 0.09	-1541390 850	-1434652 850	251.346 0.149	276 214 10
WULFENITE PbMoO <sub>4</sub>	367.138	166.10 2.09	53.86 0.10	-1051860 850	-951108 850	166.631 0.149	275 263 47
DICESIUM URANATE Cs <sub>2</sub> UO <sub>4</sub>	567.837	219.66 0.42	85.4 0.8	-1920000 3500	-1797300 3800	314.881 0.666	193 185 64 89
DISODIUM URANATE (ALPHA) Na <sub>2</sub> UO <sub>4</sub>	348.006	166.02 0.33	58.5 0.3	-1887000 3000	-1768600 3600	309.853 0.631	195 89 64 184
TRISODIUM URANIUM OXIDE Na <sub>3</sub> UO <sub>4</sub>	370.996	198.20 0.40	-2021500 4000	-1897400 4200	332.418 0.736	194 89 62 186	
SCHEELITE CaWO <sub>4</sub>	287.928	126.40 0.84	47.05 0.09	-1645150 850	-1538361 850	269.516 0.149	214 214 134
FERBERITE FeWO <sub>4</sub>	303.695	131.80 1.67	40.38 0.05	-1154780 8500	-1053880 8500	184.636 1.489	272 263 157
HUEBNERITE MnWO <sub>4</sub>	302.786	132.50 0.20	41.89 0.06				154
STOLZITE PbWO <sub>4</sub>	455.048	168.20 2.09	54.1 0.06				275
SANMARTINITE ZnWO <sub>4</sub>	313.228	119.29 0.30	39.79 0.04	-1232610 1300	-1123700 1400	196.868 0.245	153 156 153
<b>ORTHO AND RING STRUCTURE SILICATES</b>							
KYANITE Al <sub>2</sub> SiO <sub>5</sub>	162.047	83.76 0.34	44.09 0.07	-2591730 1900	-2441276 1920	427.703 0.336	120 99 205 98
ANDALUSITE Al <sub>2</sub> SiO <sub>5</sub>	162.047	93.22 0.42	51.53 0.04	-2587525 2100	-2439892 2100	427.458 0.368	120 99 205 267
SILLIMANITE Al <sub>2</sub> SiO <sub>5</sub>	162.047	96.11 0.42	49.9 0.04	-2585760 1740	-2438988 1750	427.302 0.307	120 31 205 267
MULLITE (3-2) 3Al <sub>2</sub> O <sub>3</sub> ·2SiO <sub>2</sub>	426.056	269.57 4.18	134.55 0.07	-6810421 2200	-6431286 2220	1126.739 0.389	99 99 213 267
PHENACITE Be <sub>2</sub> SiO <sub>4</sub>	110.108	64.31 0.34	37.19 0.04				120
LARNITE Ca <sub>2</sub> SiO <sub>4</sub>	172.244	127.61 0.84	51.6 0.27	-2305980 3220	-2191264 3225	383.902 0.565	120 126 45
CALCIUM OLIVINE Ca <sub>2</sub> SiO <sub>4</sub>	172.244	120.50 0.84	59.11 0.18	-2316620 3930	-2199784 3950	385.395 0.692	120 93 45 229
GEHLENITE Ca <sub>2</sub> Al <sub>2</sub> SiO <sub>7</sub>	274.206	209.80 1.64	90.24 0.09	-4007570 2820	-3808705 2900	667.272 0.508	273 93 206 11
GROSSULAR Ca <sub>3</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	450.455	255.50 0.51	125.30 0.03	-6643140 6000	-6281359 6100	1100.475 1.069	283 286 152 88
LAWSONITE CaAl <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> (OH) <sub>2</sub> ·H <sub>2</sub> O	314.242	237.61 2.09	101.32 0.12	-4879060 4600	-4525617 4700	792.873 0.823	136 9
MONTICELLITE CaMgSiO <sub>4</sub>	156.469	102.51 4.18	51.36 0.07	-2262705 3305	-2143174 3556	375.477 0.623	285 179
MERWINITE Ca <sub>3</sub> Mg(SiO <sub>4</sub> ) <sub>2</sub>	328.712	253.13 2.09	104.4 1.0	-4566790 5310	-4339403 5397	760.249 0.946	273 179 206 116
AKERMANITE Ca <sub>2</sub> MgSi <sub>2</sub> O <sub>7</sub>	272.633	209.33 2.09	92.81 0.09	-3876520 2830	-3679069 2850	644.560 0.499	273 178 206 116
TITANITE (SPHENE) CaTiSiO <sub>5</sub>	196.063	129.20 0.84	55.65 0.17	-2601400 2380	-2459855 2430	430.958 0.426	120 93 132 253
FAYALITE Fe <sub>2</sub> SiO <sub>4</sub>	203.778	148.32 1.67	46.39 0.09	-1479360 2410	-1379375 2470	241.662 0.432	252 93 190 127

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume $\text{cm}^3$	$\Delta H_{f,298}^0$ J/mol	$\Delta G_{f,298}^0$ J/mol	Log $K_f$	References $\Delta H_{f,298}^0$ $\Delta G_{f,298}^0$ S	$\Delta C_p^0$	
ORTHO AND RING STRUCTURE SILICATES									
FORSTERITE $\text{Mg}_2\text{SiO}_4$	140.694	95.19 0.84	43.79 0.03	-2170370 1325	-2051325 1345	359.385 0.236	120 93 190 128		
PYROPE $\text{Mg}_3\text{Al}_2\text{Si}_5\text{O}_{12}$	403.130	260.76 10.00	113.27 0.05	-6284620 6000	-5932412 7000	1039.341 1.226	285 31 252		
CORDIERITE $\text{Mg}_2\text{Al}_3(\text{AlSi}_5\text{O}_{18})$	584.957	407.2 3.8	233.22 0.13	-9161524 5850	-8651112 5900	1515.645 1.025	273 180 206		
TEPHROITE $\text{Mn}_2\text{SiO}_4$	201.960	163.2 4.2	48.61 0.07	-1728070 3180	-1629695 3430	285.517 0.601	120 93 160 111		
WILLEMITTE $\text{Zn}_2\text{SiO}_4$	222.844	131.38 0.84	52.42 0.08	-1636530 2469	-1522936 2510	266.813 0.440	120 126		
ZIRCON $\text{ZrSiO}_4$	183.304	84.03 1.25	39.26 0.07	-2033400 1000	-1918890 1040	336.183 0.182	120 264 115 234		
CHAIN AND BAND STRUCTURE SILICATES									
WOLLASTONITE $\text{CaSiO}_3$	116.164	82.01 0.84	39.93 0.10	-1635220 1435	-1549903 1455	271.538 0.255	120 254 240 19		
PSEUDOWOLLASTONITE $\text{CaSiO}_3$	116.164	87.45 0.84	40.08 0.14	-1628650 2594	-1544955 2636	270.669 0.462	120 116 115		
CA-AL PYROXENE $\text{CaAl}_2\text{SiO}_6$	218.126	156.00 4.00	63.5 0.09	-3275680 2761	-3103770 2971	543.770 0.521	88 286 285		
DIOPSIDE $\text{CaMg}(\text{SiO}_3)_2$	216.553	143.09 0.84	66.09 0.10	-3210760 9120	-3036554 9160	531.994 1.605	120 148 115 178		
ALPHA SPODUMENE $\text{LiAlSi}_2\text{O}_6$	186.090	129.30 0.80	58.37 0.02	-3053500 2790	-2880203 2800	504.602 0.490	211 93 211 15		
BETA SPODUMENE $\text{LiAlSi}_2\text{O}_6$	186.090	154.40 1.20	78.25 0.04	-3025300 2790	-2859487 2805	500.972 0.490	211 93 211 15		
EUCRYPTITE $\text{LiAlSiO}_4$	126.006	103.80 0.80	53.63 0.05	-2123300 1980	-2009174 1990	352.000 0.348	211 93 211 15		
CLINORHSTATITE $\text{MgSiO}_3$	100.389	67.86 0.42	31.47 0.05	-1547750 1215	-1460883 1225	255.942 0.215	120 93 115 254		
RHODONITE $\text{MnSiO}_3$	131.022	102.5 2.1	35.16 0.02	-1319350 1310	-1243081 1440	217.784 0.252	285 93 115 127 241		
JADEITE $\text{NaAl}(\text{SiO}_3)_2$	202.140	133.47 1.25	60.4 0.1	-3029400 4180	-2850834 4230	499.456 0.741	120 97 115 149		
TRENOLITE $\text{Ca}_2\text{Mg}_5[\text{Si}_8\text{O}_{22}](\text{OH})_2$	812.374	548.90 1.25	272.92 0.73	-12355080 17320	-11627910 17360	2037.170 3.041	228 270 151		
FRAMEWORK STRUCTURE SILICATES									
ANORTHITE $\text{CaAl}_2\text{Si}_2\text{O}_8$	278.211	199.30 0.30	100.79 0.05	-4229100 3125	-4003326 3145	701.371 0.551	227 286 152 93 56		
HEXAGONAL ANORTHITE $\text{CaAl}_2\text{Si}_2\text{O}_8$	278.211	214.80 1.30	99.85 0.79	-4222575 3125	-4001420 3275	701.035 0.574	136 93 257		
$\text{CaAl}_2\text{Si}_2\text{O}_8$ GLASS $\text{CaAl}_2\text{Si}_2\text{O}_8$	278.211	237.30 2.50	103.0 0.15	-4157300 3300	-3942856 3320	690.777 0.581	227 286 152 93 56		
LEONHARDITE $\text{Ca}_2\text{Al}_4\text{Si}_8\text{O}_{24} \cdot 7\text{H}_2\text{O}$	922.867	922.2 10.9	404.4 2.0	-14246460 9635	-13197115 10170	2312.078 1.782	136 93		
MICROCLINE $\text{KAlSi}_3\text{O}_8$	278.333	214.20 0.41	108.72 0.10	-3967690 3370	-3742330 3400	655.644 0.596	187 93 90 123 269		
HIGH SANIDINE $\text{KAlSi}_3\text{O}_8$	278.333	232.90 0.48	109.05 0.10	-3959560 3370	-3739776 3400	655.196 0.596	187 93 90		
$\text{KAlSi}_3\text{O}_8$ GLASS $\text{KAlSi}_3\text{O}_8$	278.333	261.60 1.78	116.5 1.0	-3914740 3370	-3703513 3500	648.843 0.613	227 93 152 269		
KALIOPHILLITE $\text{KAlSiO}_4$	158.164	133.26 1.25	59.89 0.05	-2121920 1435	-2005975 1450	351.440 0.254	120 93 201 15		

Name and formula	Formula weight g	Entropy $S_{298}^0$ J/mol·K	Molar volume $\text{cm}^3$	$\Delta H_f^0, 298$ J/mol	$\Delta G_f^0, 298$ J/mol	Log $K_f$	References S	$\Delta H_f^0$ $\Delta G_f^0$	$C_p^0$
FRAMEWORK STRUCTURE SILICATES									
LEUCITE $\text{KAlSi}_2\text{O}_6$	218.248	200.20 1.70	88.39 0.05	-3038650 2755	-2875890 2850	503.846 0.499	93 120	93 15	201
LOW ALBITE $\text{NaAlSi}_3\text{O}_8$	262.225	207.40 0.40	100.07 0.13	-3935120 3415	-3711722 3435	650.281 0.602	187 123	93 90	115 90
ANALBITE $\text{NaAlSi}_3\text{O}_8$	262.225	226.40 0.40	100.43 0.09	-3924240 3640	-3706507 3660	649.367 0.641	76 187	93 100	90
$\text{NaAlSi}_3\text{O}_8$ GLASS $\text{NaAlSi}_3\text{O}_8$	262.225	251.90 1.50	110.086 0.19	-3875460 3700	-3665330 3720	642.153 0.652	227	93	152 269
NEPHELINE $\text{NaAlSi}_3\text{O}_8$	142.055	124.35 1.25	54.16 0.06	-2092110 2420	-1977498 2450	346.449 0.363	120	93	115 229
NEPHELINE $\text{Na}_{1-x}\text{K}_{2x}\text{AlSi}_3\text{O}_8$	145.277			-2110290 2040					93 229
ANALCIME $\text{NaAlSi}_2\text{O}_6 \cdot \text{H}_2\text{O}$	220.155	234.43 2.51	97.49 0.1	-3309839 3598	-3091730 3682	541.661 0.645	120		9
DEHYDRATED ANALCIME $\text{NaAlSi}_2\text{O}_6$	202.140	175.40 1.70					136		201
SHEET STRUCTURE SILICATES									
DICKITE $\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_2$	258.162	197.07 1.25	99.3 0.07	-4118840 3766	-3796305 3807	665.100 0.667	135	93	16
KAOLINITE $\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_2$	258.162	203.05 1.25	99.52 0.26	-4120114 3975	-3799364 4017	665.636 0.704	135	93	143
HALLOYSITE $\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_2$	258.162	203.00 1.30		-4101480 2930	-3780713 3010	662.368 0.527	135	93	16
MUSCOVITE $\text{KAl}_2(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$	398.311	334.6 1.0	140.71 0.18	-5976740 3225	-5600671 3290	981.219 0.576	226	93	152 199
PHLOGOPITE $\text{KMg}_3(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$	417.262	319.66 4.18	149.91 0.36						285
FLUORPHLOGOPITE $\text{KMg}_3(\text{AlSi}_3\text{O}_{10})\text{F}_2$	421.244	336.30 2.10	146.37 0.18	-6392880 3660	-6053067 3800	1060.477 0.666	118	93	118 118
ILLITE $(\text{Al}_7\text{Mg})(\text{Si}_{14}\text{Al}_2)\text{O}_{40}(\text{OH})_8$	1553.675	1104.20 0.60							226
TALC $\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$	379.268	260.83 0.63	136.25 0.26	-5915900 4330	-5536048 4350	969.897 0.762	228	93	151 11
PYROPHYLLITE $\text{Al}_2\text{Si}_4\text{O}_{10}(\text{OH})_2$	360.317	239.40 0.40	127.82 0.29	-5639800 3950	-5265884 3960	922.567 0.694	226	286	152 139
CHRYSOTILE $\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_4$	277.113	221.30 0.80	108.5 0.6	-4361660 3480	-4034024 3500	706.747 0.613	128	93	128 128

SILVER (REFERENCE STATE)

FORMULA WEIGHT 107.868

Ag: Face-centered cubic crystals 298.15 to melting point 1234 K. Liquid 1234 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	42.55	42.55	25.40	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.530	50.08	43.55	25.87	.000	.000	.000
500	10.444	55.90	45.46	26.33	.000	.000	.000
600	13.135	60.75	47.61	26.88	.000	.000	.000
700	15.144	64.94	49.80	27.52	.000	.000	.000
800	16.736	68.66	51.92	28.24	.000	.000	.000
900	18.058	72.04	53.98	29.03	.000	.000	.000
1000	19.196	75.14	55.94	29.86	.000	.000	.000
1100	20.205	78.02	57.82	30.73	.000	.000	.000
1200	21.120	80.74	59.62	31.64	.000	.000	.000
1234	21.411	81.73	60.32	31.96	.000	.000	.000
1234	30.566	90.88	60.32	33.47	.000	.000	.000
1300	30.714	92.52	61.81	33.47	.000	.000	.000
1400	30.911	95.00	64.09	33.47	.000	.000	.000
1500	31.082	97.31	66.23	33.47	.000	.000	.000
1600	31.231	99.47	68.24	33.47	.000	.000	.000
1700	31.363	101.50	70.14	33.47	.000	.000	.000
1800	31.480	103.41	71.93	33.47	.000	.000	.000

MELTING POINT	1234 K	BOILING POINT	2436 K
ENTHALPY OF MELTING	11.945 kJ	ENTHALPY OF VAPORIZATION	254.303 kJ
$H_{298}^0 - H_0^0$	5.745 kJ	MOLAR VOLUME	1.0272 J/bar 10.272 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 11.255 + 1.1692 \times 10^{-2} T + 2.2534 \times 10^{-2} T^{0.5} - 2.1236 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1234 K)

REFERENCE 107

35

COMPILED  
4-10-76

ALUMINUM (REFERENCE STATE)

FORMULA WEIGHT 26.982

Al: Face-centered cubic crystals 298.15 to melting point 933 K. Liquid 933 to 1800 K.

TEMP.	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	FORMATION FROM THE ELEMENTS		
					ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	28.35	28.35	24.31	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	6.372	35.70	29.33	25.65	.000	.000	.000
500	10.338	41.54	31.20	26.73	.000	.000	.000
600	13.165	46.51	33.34	27.89	.000	.000	.000
700	15.363	50.91	35.55	29.25	.000	.000	.000
800	17.195	54.92	37.72	30.83	.000	.000	.000
900	18.810	58.65	39.84	32.67	.000	.000	.000
933.25	19.321	60.02	40.70	33.34	.000	.000	.000
933.25	30.888	71.59	40.70	31.75	.000	.000	.000
1000	30.946	73.61	42.66	31.75	.000	.000	.000
1100	31.019	76.64	45.62	31.75	.000	.000	.000
1200	31.081	79.40	48.32	31.75	.000	.000	.000
1300	31.132	81.95	50.82	31.75	.000	.000	.000
1400	31.177	84.30	53.12	31.75	.000	.000	.000
1500	31.215	86.49	55.27	31.75	.000	.000	.000
1600	31.249	88.54	57.29	31.75	.000	.000	.000
1700	31.279	90.46	59.18	31.75	.000	.000	.000
1800	31.306	92.28	60.97	31.75	.000	.000	.000

MELTING POINT 933.25 K BOILING POINT 2793 K  
 ENTHALPY OF MELTING 10.711 kJ ENTHALPY OF VAPORIZATION 290.775 kJ  
 $H_{298}^0 - H_0^0$  4.565 kJ MOLAR VOLUME 0.9999 J/bar  
 9.999 cm<sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 27.237 - 6.5674 \times 10^{-3} T + 1.4310 \times 10^{-5} T^2 - 1.9916 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 933.25 K)

REFERENCE 107 35

COMPILED  
4-10-76

ARGON (REFERENCE STATE)

FORMULA WEIGHT 39.948

At: Ideal gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	154.84	154.84	20.79	0.000	0.000	0.000
UNCERTAINTY		0.02	0.02				
400	5.292	160.95	155.66	20.79	.000	.000	.000
500	8.392	165.59	157.20	20.79	.000	.000	.000
600	10.457	169.38	158.92	20.79	.000	.000	.000
700	11.933	172.58	160.65	20.79	.000	.000	.000
800	13.040	175.36	162.32	20.79	.000	.000	.000
900	13.900	177.80	163.90	20.79	.000	.000	.000
1000	14.589	179.99	165.40	20.79	.000	.000	.000
1100	15.152	181.98	166.83	20.79	.000	.000	.000
1200	15.622	183.78	168.16	20.79	.000	.000	.000
1300	16.019	185.45	169.43	20.79	.000	.000	.000
1400	16.359	186.99	170.63	20.79	.000	.000	.000
1500	16.655	188.42	171.77	20.79	.000	.000	.000
1600	16.912	189.76	172.85	20.79	.000	.000	.000
1700	17.141	191.02	173.88	20.79	.000	.000	.000
1800	17.343	192.21	174.87	20.79	.000	.000	.000

MELTING POINT	83.80 K	BOILING POINT	87.30 K
ENTHALPY OF MELTING	1.176 kJ	ENTHALPY OF VAPORIZATION	6.561 kJ
$H_{298}^0 - H_0^0$	6.197 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE	107	35	COMPILED 3-11-76
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ARSENIC (REFERENCE STATE)

FORMULA WEIGHT 74.922

As: Rhombohedral crystals 298.15 to sublimation point 875 K. Ideal  
tetraatomic gas 875 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	35.69	35.69	24.65	0.000	0.000	0.000
UNCERTAINTY		0.84	0.84				
400	6.375	43.04	36.66	25.38	.000	.000	.000
500	10.234	48.77	38.54	25.96	.000	.000	.000
600	12.902	53.55	40.65	26.51	.000	.000	.000
700	14.883	57.68	42.80	27.05	.000	.000	.000
800	16.439	61.33	44.89	27.60	.000	.000	.000
875	17.317	63.82	46.51	28.03	.000	.000	.000
875	57.114	103.62	46.51	20.60	.000	.000	.000
900	56.141	104.14	48.00	20.61	.000	.000	.000
1000	52.590	106.31	53.72	20.64	.000	.000	.000
1100	49.686	108.28	58.59	20.67	.000	.000	.000
1200	47.269	110.08	62.81	20.69	.000	.000	.000

MELTING POINT	K	BOILING POINT	875 K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	34.828 kJ
$H_{298}^0 - H_0^0$	5.130 kJ	MOLAR VOLUME	1.2963 J/bar 12.963 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 20.845 + 6.3265 \times 10^{-3} T + 52.398 T^{-0.5} - 9.8777 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 875 K)

$$C_P^0 = 21.139 - 9.1839 \times 10^{-5} T - 9.1807 T^{-0.5} - 1.1342 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 875 - 1200 K)

REFERENCE 107 107

COMPILED  
5-15-76

GOLD (REFERENCE STATE)

FORMULA WEIGHT 196.966

Au: Face-centered cubic crystals 298.15 to melting point 1336.15 K. Liquid  
1336.15 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	S <sub>T</sub> <sup>0</sup>	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	C <sub>p</sub> <sup>0</sup>	ENTHALPY	FREE ENERGY	
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	47.49	47.49	25.32	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.512	55.00	48.49	25.88	.000	.000	.000
500	10.428	60.82	50.39	26.27	.000	.000	.000
600	13.093	65.64	52.55	26.57	.000	.000	.000
700	15.043	69.76	54.72	26.92	.000	.000	.000
800	16.554	73.38	56.83	27.36	.000	.000	.000
900	17.784	76.63	58.85	27.94	.000	.000	.000
1000	18.835	79.61	60.77	28.67	.000	.000	.000
1100	19.769	82.39	62.62	29.58	.000	.000	.000
1200	20.631	85.01	64.38	30.67	.000	.000	.000
1300	21.452	87.51	66.06	31.95	.000	.000	.000
1336.15	21.805	88.55	66.74	32.47	.000	.000	.000
1336.15	31.199	97.94	66.74	33.54	.000	.000	.000
1400	31.231	99.34	68.11	32.75	.000	.000	.000
1500	31.275	101.54	70.26	31.49	.000	.000	.000
1600	31.252	103.54	72.29	30.81	.000	.000	.000
1700	31.212	105.39	74.18	30.81	.000	.000	.000
1800	31.189	107.15	75.96	30.81	.000	.000	.000

MELTING POINT	1336.15 K	BOILING POINT	3130 K
ENTHALPY OF MELTING	12.364 kJ	ENTHALPY OF VAPORIZATION	335.054 kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	6.017 kJ	MOLAR VOLUME	1.0215 J/bar 10.215 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATIONS

$$C_p^0 = 41.968 - 1.7696 \times 10^{-2} T + 1.1232 \times 10^{-5} T^2 - 2.1606 \times 10^2 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1336.15 K)

$$C_p^0 = -1.3492 \times 10^4 + 3.7585 T - 5.2249 \times 10^{-4} T^2 + 3.8267 \times 10^5 T^{-0.5}$$

-1.8431 × 10<sup>9</sup> T<sup>-2</sup>  
EQUATION VALID FROM 1336.15 - 1800 K)

REFERENCE 107 107

COMPILED  
5-03-76



BORON (REFERENCE STATE)

FORMULA WEIGHT 10.810

B: Rhombohedral crystals 298.15 to melting point 2300 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol
298.15	0.000	5.90	5.90	11.09	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	3.400	9.79	6.39	15.49	.000	.000	.000
500	6.142	13.60	7.46	18.53	.000	.000	.000
600	8.393	17.17	8.78	20.66	.000	.000	.000
700	10.261	20.48	10.22	22.21	.000	.000	.000
800	11.832	23.53	11.70	23.39	.000	.000	.000
900	13.170	26.34	13.17	24.32	.000	.000	.000
1000	14.323	28.94	14.62	25.08	.000	.000	.000
1100	15.331	31.36	16.03	25.73	.000	.000	.000
1200	16.222	33.62	17.40	26.31	.000	.000	.000
1300	17.020	35.75	18.73	26.86	.000	.000	.000
1400	17.742	37.76	20.02	27.40	.000	.000	.000
1500	18.405	39.67	21.27	27.95	.000	.000	.000
1600	19.019	41.49	22.47	28.52	.000	.000	.000
1700	19.595	43.24	23.65	29.11	.000	.000	.000
1800	20.141	44.92	24.78	29.75	.000	.000	.000

MELTING POINT	2300 K	BOILING POINT	4275 K
ENTHALPY OF MELTING	22.552 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	1.222 kJ	MOLAR VOLUME	0.4386 J/bar 4.386 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

HEAT CAPACITY EQUATION

$$C_P^0 = 66.520 - 1.7059 \times 10^{-2} T + 4.9067 \times 10^{-6} T^2 - 9.3527 \times 10^{-9} T^{-0.5} + 2.8390 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107

107

COMPILED  
5-04-76

BARIUM (REFERENCE STATE)

FORMULA WEIGHT 137.330

Ba: Body-centered cubic crystals 298.15 to second-order lambda-anomaly in heat capacity at 582.53 K. Beta crystals 582.53 to second-order lambda-anomaly in heat capacity at 768.13 K. Gamma crystals 768.13 to melting point 1002 K. Liquid 1002 to boiling point 2169 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	62.42	62.42	28.09	0.000	0.000	0.000
UNCERTAINTY		0.84	0.84				
400	7.677	71.24	63.56	33.23	.000	.000	.000
500	13.774	79.72	65.94	43.74	.000	.000	.000
582.53	18.190	86.71	68.52	54.43	.000	.000	.000
582.53	18.614	87.13	68.52	32.47	.000	.000	.000
600	19.183	88.16	68.97	33.94	.000	.000	.000
700	21.894	94.02	72.13	42.36	.000	.000	.000
768.13	23.640	98.02	74.38	48.10	.000	.000	.000
768.13	23.964	98.34	74.38	39.07	.000	.000	.000
800	24.565	99.81	75.24	39.07	.000	.000	.000
900	26.173	104.41	78.24	39.07	.000	.000	.000
1000	27.464	108.52	81.06	39.07	.000	.000	.000
1002	27.876	109.34	81.46	39.07	.000	.000	.000
1002	35.610	117.07	81.46	40.62	.000	.000	.000
1100	36.127	120.60	84.48	40.37	.000	.000	.000
1200	36.568	124.20	87.64	40.12	.000	.000	.000
1300	36.864	127.44	90.58	39.86	.000	.000	.000
1400	37.079	130.38	93.30	39.61	.000	.000	.000
1500	37.199	133.08	95.88	39.36	.000	.000	.000
1600	37.295	135.58	98.28	39.10	.000	.000	.000
1700	37.371	137.92	100.55	38.85	.000	.000	.000
1800	37.440	140.13	102.69	38.60	.000	.000	.000

MELTING POINT	1002 K	BOILING POINT	2169 K
ENTHALPY OF MELTING	7.749 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	6.912 kJ	MOLAR VOLUME	3.8210 J/bar 38.210 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 43.154 - 2.5318 \times 10^{-3} T$$

(EQUATION VALID FROM 1002 - 1800 K)

REFERENCE 107 107

COMPILED  
7-27-76

BERYLLIUM (REFERENCE STATE) FORMULA WEIGHT 9.012

Be: Hexagonal close packed crystals 298.15 to 1527 K. Beta crystals 1527 to melting point 1560 K. Liquid 1560 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	9.54	9.54	16.41	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	4.652	14.88	10.23	19.81	.000	.000	.000
500	7.906	19.54	11.63	21.90	.000	.000	.000
600	10.368	23.68	13.31	23.39	.000	.000	.000
700	12.314	27.37	15.06	24.55	.000	.000	.000
800	13.907	30.72	16.81	25.54	.000	.000	.000
900	15.250	33.78	18.53	26.44	.000	.000	.000
1000	16.411	36.61	20.20	27.28	.000	.000	.000
1100	17.438	39.25	21.81	28.12	.000	.000	.000
1200	18.363	41.73	23.37	28.97	.000	.000	.000
1300	19.213	44.08	24.87	29.85	.000	.000	.000
1400	20.005	46.33	26.33	30.77	.000	.000	.000
1500	20.755	48.48	27.73	31.74	.000	.000	.000
1527	20.964	49.00	28.03	31.84	.000	.000	.000
1527	22.638	50.67	28.03	32.22	.000	.000	.000
1560	22.840	51.34	28.49	32.22	.000	.000	.000
1560	30.669	59.16	28.49	29.46	.000	.000	.000
1600	30.638	60.00	29.36	29.45	.000	.000	.000
1700	30.569	61.79	31.22	29.45	.000	.000	.000
1800	30.507	63.47	32.96	29.45	.000	.000	.000

MELTING POINT	1560 K	BOILING POINT	2745 K
ENTHALPY OF MELTING	12.213 kJ	ENTHALPY OF VAPORIZATION	326.519 kJ
$H_{298}^0 - H_0^0$	1.954 kJ	MOLAR VOLUME	0.4880 J/bar 4.880 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 43.418 - 7.7662 \times 10^{-3} T + 4.7111 \times 10^{-6} T^2 - 4.0972 \times 10^{-9} T^3 - 1.2262 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1527 K)

REFERENCE 107 107

COMPILED  
5-03-76

## BISMUTH (REFERENCE STATE)

FORMULA WEIGHT 208.980

Bi: Rhombohedral crystals 298.15 to melting point 544.5 K. Liquid 544.5 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	56.74	56.74	25.41	0.000	0.000	0.000
UNCERTAINTY		0.42	0.42				
400	6.607	64.36	57.75	26.62	.000	.000	.000
500	10.800	70.50	59.70	28.66	.000	.000	.000
544.52	12.393	73.40	61.01	29.83	.000	.000	.000
544.52	33.140	94.15	61.01	30.48	.000	.000	.000
600	32.763	96.64	63.88	29.61	.000	.000	.000
700	32.236	101.13	68.89	28.61	.000	.000	.000
800	31.742	104.90	73.16	28.02	.000	.000	.000
900	31.308	108.18	76.87	27.67	.000	.000	.000
1000	30.931	111.08	80.15	27.45	.000	.000	.000
1100	30.608	113.69	83.08	27.31	.000	.000	.000
1200	30.330	116.07	85.74	27.24	.000	.000	.000
1300	30.090	118.25	88.16	27.19	.000	.000	.000
1400	29.882	120.26	90.38	27.17	.000	.000	.000
1500	29.701	122.13	92.43	27.17	.000	.000	.000
1600	29.544	123.89	94.35	27.18	.000	.000	.000
1700	29.405	125.54	96.14	27.19	.000	.000	.000
1800	29.283	127.09	97.81	27.21	.000	.000	.000

MELTING POINT	544.52 K	BOILING POINT	1835 K
ENTHALPY OF MELTING	11.297 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	6.427 kJ	MOLAR VOLUME	2.1309 J/bar 21.309 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATIONS

$$C_p^0 = 26.852 - 1.7289 \times 10^{-2} T + 4.1802 \times 10^{-5} T^2$$

(EQUATION VALID FROM 298 - 544.52 K)

$$C_p^0 = 29.827 - 1.3600 \times 10^{-2} T^{0.5} + 1.9213 \times 10^{-6} T^{-2}$$

EQUATION VALID FROM 544.52 - 1800 K)

REFERENCE	76	107	COMPILED 4-10-76
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BROMINE (REFERENCE STATE)

FORMULA WEIGHT 159.808

Br<sub>2</sub>: Liquid 298.15 to boiling point 332 K. Ideal diatomic gas 332 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	152.32	152.32	36.06	0.000	0.000	0.000
UNCERTAINTY		0.04	0.04				
332	7.837	160.36	152.53	96.69	.000	.000	.000
332	96.694	249.33	152.53	36.33	.000	.000	.000
400	86.535	256.16	169.63	36.73	.000	.000	.000
500	76.618	264.40	187.78	37.07	.000	.000	.000
600	70.040	271.17	201.13	37.29	.000	.000	.000
700	65.371	276.93	211.56	37.45	.000	.000	.000
800	61.886	281.94	220.05	37.57	.000	.000	.000
900	59.184	286.36	227.18	37.67	.000	.000	.000
1000	57.032	290.33	233.30	37.76	.000	.000	.000
1100	55.278	293.93	238.65	37.84	.000	.000	.000
1200	53.820	297.22	243.40	37.91	.000	.000	.000
1300	52.593	300.25	247.66	37.98	.000	.000	.000
1400	51.544	303.06	251.51	38.05	.000	.000	.000
1500	50.640	305.68	255.04	38.11	.000	.000	.000
1600	49.852	308.13	258.28	38.18	.000	.000	.000
1700	49.159	310.44	261.28	38.24	.000	.000	.000
1800	48.546	312.62	264.07	38.31	.000	.000	.000

MELTING POINT	265.90 K	BOILING POINT	332 K
ENTHALPY OF MELTING	10.573 kJ	ENTHALPY OF VAPORIZATION	29.556 kJ
$H_{298}^0 - H_0^0$	24.520 kJ	MOLAR VOLUME	5.4580 J/bar 54.580 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 38.426 + 1.3663 \times 10^{-7} T^2 - 22.423 T^{-0.5} - 9.5885 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 332 - 1800 K)

REFERENCE 107 107 COMPILED 3-11-76

CARBON (REFERENCE STATE) FORMULA WEIGHT 12.011

C: Graphite 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	5.74	5.74	8.53	0.000	0.000	0.000
UNCERTAINTY		0.01	0.01				
400	2.610	8.73	6.12	11.92	.000	.000	.000
500	4.762	11.70	6.94	14.70	.000	.000	.000
600	6.607	14.58	7.97	16.86	.000	.000	.000
700	8.196	17.31	9.11	18.53	.000	.000	.000
800	9.570	19.87	10.30	19.81	.000	.000	.000
900	10.767	22.26	11.49	20.82	.000	.000	.000
1000	11.812	24.50	12.69	21.60	.000	.000	.000
1100	12.732	26.59	13.86	22.23	.000	.000	.000
1200	13.544	28.54	15.00	22.72	.000	.000	.000
1300	14.266	30.38	16.11	23.12	.000	.000	.000
1400	14.910	32.11	17.20	23.44	.000	.000	.000
1500	15.488	33.73	18.24	23.70	.000	.000	.000
1600	16.008	35.27	19.26	23.92	.000	.000	.000
1700	16.479	36.72	20.24	24.11	.000	.000	.000
1800	16.908	38.11	21.20	24.27	.000	.000	.000

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	1.050 kJ	MOLAR VOLUME	0.5298 J/bar 5.298 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 63.160 - 1.1468 \times 10^{-2} T + 1.8079 \times 10^{-6} T^2 - 1.0323 \times 10^{-9} T^3 + 7.4807 \times 10^{-13} T^4$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107 COMPILED  
3-11-76

DIAMOND FORMULA WEIGHT 12.011

C: Diamond 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	2.38	2.38	6.13	1.895	2.900	-0.508
UNCERTAINTY		0.01	0.01		0.042	0.084	0.015
400	2.087	4.76	2.67	10.23	1.686	3.274	-0.428
500	4.066	7.42	3.35	13.59	1.547	3.687	-0.385
600	5.873	10.13	4.26	16.12	1.455	4.125	-0.359
700	7.479	12.76	5.28	18.01	1.393	4.578	-0.342
800	8.890	15.27	6.38	19.47	1.351	5.031	-0.328
900	10.132	17.63	7.50	20.64	1.324	5.491	-0.319
1000	11.233	19.86	8.63	21.62	1.316	5.956	-0.311
1100	12.218	21.96	9.74	22.50	1.330	6.423	-0.305
1200	13.110	23.95	10.84	23.34	1.374	6.882	-0.300
1300	13.929	25.86	11.93	24.18	1.457	7.333	-0.295
1400	14.693	27.68	12.99	25.07	1.591	7.793	-0.291
1500	15.416	29.44	14.02	26.02	1.787	8.222	-0.286
1600	16.111	31.15	15.04	27.06	2.059	8.651	-0.282
1700	16.788	32.83	16.04	28.21	2.419	9.032	-0.278
1800	17.457	34.47	17.01	29.49	2.883	9.435	-0.274

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	0.523 kJ	MOLAR VOLUME	0.3417 J/bar 3.417 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 98.445 - 3.6554 \times 10^{-2} T + 1.0977 \times 10^{-5} T^2 - 1.6590 \times 10^{-8} T^{-0.5} + 1.2166 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107 87 COMPILED 5-19-76

CALCIUM (REFERENCE STATE) FORMULA WEIGHT 40.080

Ca: Alpha crystals (face-centered cubic) 298.15 to 720 K. Beta crystals (body-centered cubic) 720 to melting point 1112 K. Liquid 1112 to boiling point 1755 K. Ideal monatomic gas 1755 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	41.63	41.63	25.30	0.000	0.000	0.000
UNCERTAINTY		0.42	0.42				
400	6.552	49.19	42.64	26.26	.000	.000	.000
500	10.628	55.19	44.56	27.68	.000	.000	.000
600	13.620	60.40	46.78	29.55	.000	.000	.000
700	16.056	65.12	49.06	31.85	.000	.000	.000
720	16.462	66.38	49.92	32.35	.000	.000	.000
720	17.367	67.29	49.92	29.34	.000	.000	.000
800	19.101	70.56	51.46	32.65	.000	.000	.000
900	20.836	74.65	53.81	36.77	.000	.000	.000
1000	22.636	78.74	56.10	40.90	.000	.000	.000
1100	24.485	82.83	58.35	45.03	.000	.000	.000
1112	24.709	83.50	58.79	45.52	.000	.000	.000
1112	32.384	91.17	58.79	29.29	.000	.000	.000
1200	32.157	93.23	61.07	29.29	.000	.000	.000
1300	31.937	95.57	63.63	29.29	.000	.000	.000
1400	31.748	97.74	65.99	29.29	.000	.000	.000
1500	31.583	99.76	68.18	29.29	.000	.000	.000
1600	31.440	101.65	70.21	29.29	.000	.000	.000
1700	31.314	103.43	72.12	29.29	.000	.000	.000
1755	31.251	104.18	72.93	29.29	.000	.000	.000
1755	118.815	191.75	72.93	20.83	.000	.000	.000
1800	116.479	192.25	75.77	20.84	.000	.000	.000

MELTING POINT	1112 K	BOILING POINT	1755 K
ENTHALPY OF MELTING	8.535 kJ	ENTHALPY OF VAPOORIZATION	153.675 kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	5.707 kJ	MOLAR VOLUME	2.6190 J/bar 26.190 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

#### HEAT CAPACITY EQUATIONS

$$C_P^0 = 10.786 + 8.7646 \times 10^{-3} T + 1.4996 \times 10^{-5} T^2 + 2.0745 \times 10^{-8} T^{-0.5} - 1.2877 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 720 K)

$$C_P^0 = -0.34497 + 4.1256 \times 10^{-2} T - 8.5285 \times 10^3 T^{-2}$$

(EQUATION VALID FROM 720 - 1112 K)

REFERENCE 107 107

COMPILED  
4-10-76



CADMIUM (REFERENCE STATE) FORMULA WEIGHT 112.410

Cd: Hexagonal close packed crystals 298.15 to melting point 594.18 K. Liquid  
594.18 to boiling point 1039 K. Ideal monatomic gas 1039 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	51.80	51.80	25.98	0.000	0.000	0.000
UNCERTAINTY							
		0.17	0.17				
400	6.760	59.59	52.83	27.14	.000	.000	.000
500	10.958	65.78	54.82	28.37	.000	.000	.000
594.18	13.811	70.79	56.98	29.53	.000	.000	.000
594.18	24.232	81.21	56.98	29.71	.000	.000	.000
600	24.285	81.48	57.19	29.71	.000	.000	.000
700	25.059	86.06	61.00	29.71	.000	.000	.000
800	25.640	90.03	64.39	29.71	.000	.000	.000
900	26.092	93.53	67.44	29.71	.000	.000	.000
1000	26.453	96.66	70.21	29.71	.000	.000	.000
1039	26.529	97.97	71.44	29.71	.000	.000	.000
1039	122.455	193.90	71.44	20.79	.000	.000	.000
1100	116.817	194.88	78.06	20.79	.000	.000	.000
1200	108.814	196.69	87.88	20.79	.000	.000	.000
1300	102.043	198.35	96.31	20.79	.000	.000	.000
1400	96.239	199.89	103.65	20.79	.000	.000	.000
1500	91.209	201.33	110.12	20.79	.000	.000	.000
1600	86.807	202.67	115.86	20.79	.000	.000	.000
1700	82.924	203.93	121.01	20.79	.000	.000	.000
1800	79.472	205.12	125.65	20.79	.000	.000	.000

MELTING POINT	594.18 K	BOILING POINT	1039 K
ENTHALPY OF MELTING	6.192 kJ	ENTHALPY OF VAPORIZATION	99.667 kJ
$H_{298}^0 - H_0^0$	6.251 kJ	MOLAR VOLUME	1.3005 J/bar 13.005 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_p^0 = 3.8115 \times 10^{-2} T - 1.4336 \times 10^{-5} T^2 + 3.0044 \times 10^2 T^{-0.5} - 1.3402 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 594.18 K)

REFERENCE 107 107

COMPILED  
5-06-76

CERIUM (REFERENCE STATE)

FORMULA WEIGHT 140.120

Ce: Alpha crystals (face-centered cubic) 298.15 to 999 K. Beta crystals 999 to melting point 1071 K. Liquid 1071 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS					ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log $K_f$
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K				
298.15	0.000	69.46	69.46	26.93	0.000	0.000	0.000	
UNCERTAINTY		8.37	8.37					
400	7.030	77.56	70.53	28.29	.000	.000	.000	
500	11.422	84.03	72.61	29.70	.000	.000	.000	
600	14.592	89.57	74.98	31.20	.000	.000	.000	
700	17.076	94.50	77.42	32.77	.000	.000	.000	
800	19.139	98.98	79.84	34.40	.000	.000	.000	
900	20.927	103.13	82.20	36.07	.000	.000	.000	
999	22.344	106.81	84.47	37.76	.000	.000	.000	
999	25.452	109.92	84.47	37.61	.000	.000	.000	
1000	25.519	110.01	84.49	37.61	.000	.000	.000	
1071	26.318	112.65	86.33	37.61	.000	.000	.000	
1071	31.416	117.75	86.33	37.70	.000	.000	.000	
1100	31.582	118.70	87.12	37.70	.000	.000	.000	
1200	32.092	121.98	89.89	37.70	.000	.000	.000	
1300	32.523	124.99	92.47	37.70	.000	.000	.000	
1400	32.892	127.79	94.90	37.70	.000	.000	.000	
1500	33.213	130.39	97.18	37.70	.000	.000	.000	
1600	33.493	132.82	99.33	37.70	.000	.000	.000	
1700	33.741	135.11	101.37	37.70	.000	.000	.000	
1800	33.960	137.26	103.30	37.70	.000	.000	.000	

MELTING POINT	1071 K	BOILING POINT	K
ENTHALPY OF MELTING	5.460 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	7.280 kJ	MOLAR VOLUME	2.0770 J/bar 20.770 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 14.017 + 1.9292 \times 10^{-2} T + 1.4469 \times 10^{-2} T^{-0.5} - 1.0802 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 999 K)

REFERENCE 107 107

COMPILED  
4-26-76

CHLORINE (REFERENCE STATE)

FORMULA WEIGHT 70.906

Cl<sub>2</sub>: Ideal diatomic gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	223.08	223.08	33.98	0.000	0.000	0.000
UNCERTAINTY		0.04	0.04				
400	8.830	233.26	224.43	35.26	.000	.000	.000
500	14.198	241.22	227.02	36.03	.000	.000	.000
600	17.882	247.84	229.96	36.54	.000	.000	.000
700	20.574	253.50	232.93	36.88	.000	.000	.000
800	22.629	258.44	235.81	37.13	.000	.000	.000
900	24.251	262.82	238.57	37.31	.000	.000	.000
1000	25.565	266.76	241.19	37.45	.000	.000	.000
1100	26.650	270.34	243.69	37.56	.000	.000	.000
1200	27.563	273.61	246.05	37.65	.000	.000	.000
1300	28.342	276.63	248.29	37.73	.000	.000	.000
1400	29.016	279.42	250.40	37.80	.000	.000	.000
1500	29.603	282.03	252.43	37.87	.000	.000	.000
1600	30.123	284.48	254.36	37.95	.000	.000	.000
1700	30.585	286.78	256.19	38.03	.000	.000	.000
1800	31.001	288.96	257.96	38.11	.000	.000	.000

MELTING POINT	172.16 K	BOILING POINT	239.10 K
ENTHALPY OF MELTING	6.406 kJ	ENTHALPY OF VAPORIZATION	20.410 kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	9.180 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

HEAT CAPACITY EQUATION

$$C_P^0 = 46.956 - 4.0158 \times 10^{-3} T + 9.9274 \times 10^{-7} T^2 - 2.0495 \times 10^{-10} T^4$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 35 COMPILED 3-11-76

COBALT (REFERENCE STATE)

FORMULA WEIGHT 58.933

Co: Alpha crystals (hexagonal close packed) 298.15 to 700 K. Beta crystals (face-centered cubic) 700 to melting point 1768 K. Liquid 1768 to 1800 K. Curie point at 1394 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	30.04	30.04	24.31	0.000	0.000	0.000
UNCERTAINTY		0.42	0.42				
400	6.542	37.58	31.04	26.56	.000	.000	.000
500	10.710	43.68	32.97	28.19	.000	.000	.000
600	13.752	48.96	35.21	29.70	.000	.000	.000
700	16.138	53.64	37.49	31.05	.000	.000	.000
700	16.780	54.27	37.49	30.58	.000	.000	.000
800	18.625	58.50	39.88	32.58	.000	.000	.000
900	20.283	62.45	42.17	34.55	.000	.000	.000
1000	21.820	66.20	44.38	36.85	.000	.000	.000
1100	23.313	69.84	46.53	39.77	.000	.000	.000
1200	24.834	73.46	48.63	43.52	.000	.000	.000
1300	26.446	77.12	50.67	48.26	.000	.000	.000
1394	28.150	80.67	52.52	53.70	.000	.000	.000
1400	28.236	80.88	52.64	44.22	.000	.000	.000
1500	29.115	83.72	54.60	39.75	.000	.000	.000
1600	29.727	86.23	56.50	38.28	.000	.000	.000
1700	30.213	88.53	58.32	37.78	.000	.000	.000
1768	30.500	90.00	59.50	37.74	.000	.000	.000
1768	39.660	99.16	59.50	40.50	.000	.000	.000
1800	39.678	99.98	60.30	40.50	.000	.000	.000

MELTING POINT	1768 K	BOILING POINT	3201 K
ENTHALPY OF MELTING	16.192 kJ	ENTHALPY OF VAPORIZATION	376.551 kJ
$H_{298}^0 - H_0^0$	4.766 kJ	MOLAR VOLUME	6.6670 J/bar 6.670 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 4.1844 \times 10^{-2} T - 1.6498 \times 10^{-5} T^2 + 2.6875 \times 10^2 T^{-0.5} - 1.5646 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 700 K)

$$C_P^0 = 2.8332 \times 10^2 - 0.19791 T + 7.9727 \times 10^{-5} T^2 - 4.0569 \times 10^3 T^{-0.5}$$

(EQUATION VALID FROM 700 - 1394 K)

REFERENCE 107 107

COMPILED  
5-12-76

CHROMIUM (REFERENCE STATE)

FORMULA WEIGHT 51.996

Cr: Body-centered cubic crystals 298.15 to melting point 2130 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	23.64	23.64	23.37	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.257	30.85	24.59	25.45	.000	.000	.000
500	10.206	36.64	26.43	26.48	.000	.000	.000
600	12.993	41.55	28.56	27.38	.000	.000	.000
700	15.117	45.85	30.73	28.36	.000	.000	.000
800	16.841	49.70	32.86	29.47	.000	.000	.000
900	18.313	53.25	34.94	30.73	.000	.000	.000
1000	19.624	56.56	36.94	32.13	.000	.000	.000
1100	20.830	59.69	38.86	33.67	.000	.000	.000
1200	21.969	62.69	40.72	35.33	.000	.000	.000
1300	23.065	65.59	42.53	37.12	.000	.000	.000
1400	24.136	68.41	44.27	39.01	.000	.000	.000
1500	25.193	71.17	45.98	41.01	.000	.000	.000
1600	26.247	73.88	47.63	43.12	.000	.000	.000
1700	27.304	76.56	49.26	45.32	.000	.000	.000
1800	28.368	79.21	50.84	47.61	.000	.000	.000

MELTING POINT	2130 K	BOILING POINT	2945 K
ENTHALPY OF MELTING	16.933 kJ	ENTHALPY OF VAPORIZATION	344.314 kJ
$H_{298}^0 - H_0^0$	4.058 kJ	MOLAR VOLUME	0.7231 J/bar 7.231 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.3869 \times 10^{-2} T + 3.4687 \times 10^{-6} T^2 + 4.9535 \times 10^{-9} T^{-0.5} - 8.6742 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
5-19-76

CESIUM (REFERENCE STATE) FORMULA WEIGHT 132.905

Cs: Body-centered cubic crystals 298.15 to melting point 301.55 K. Liquid  
301.55 to boiling point 942 K. Ideal monatomic gas 942 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K			
298.15	0.000	85.23	85.23	32.18	0.000	0.000	0.000
UNCERTAINTY		0.40	0.40				
301.55	0.361	85.43	85.06	32.46	.000	.000	.000
301.55	7.298	92.37	85.06	42.75	.0000	.000	.000
400	15.175	103.68	88.50	35.94	.000	.000	.000
500	18.746	111.07	92.32	30.45	.000	.000	.000
600	20.390	116.30	95.91	27.14	.000	.000	.000
700	21.250	120.37	99.12	26.06	.000	.000	.000
800	21.896	123.90	102.00	27.14	.000	.000	.000
900	22.636	127.26	104.62	30.31	.000	.000	.000
942	23.024	128.69	105.67	32.35	.000	.000	.000
942	93.844	199.51	105.67	20.79	.000	.000	.000
1000	89.606	200.75	111.14	20.79	.000	.000	.000
1100	83.350	202.73	119.38	20.79	.000	.000	.000
1200	78.137	204.54	126.40	20.79	.000	.000	.000
1300	73.726	206.21	132.48	20.80	.000	.000	.000
1400	69.945	207.75	137.80	20.80	.000	.000	.000
1500	66.668	209.15	142.48	20.80	.000	.000	.000
1600	63.800	210.50	146.70	20.80	.000	.000	.000
1700	61.270	211.77	150.50	20.80	.000	.000	.000
1800	59.021	212.97	153.95	20.81	.000	.000	.000

MELTING POINT	301.55 K	BOILING POINT	942 K
ENTHALPY OF MELTING	2.092 kJ	ENTHALPY OF VAPORIZATION	67.712 kJ
$H_{298}^0 - H_0^0$	7.711 kJ	MOLAR VOLUME	6.9730 J/bar 69.730 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

#### HEAT CAPACITY EQUATIONS

$$C_p^0 = -9.2360 \times 10^{-2} T + 8.6400 \times 10^{-5} T^2 + 1.3549 \times 10^3 T^{-0.5} - 1.3896 \times 10^6 T^{-2}$$

EQUATION VALID FROM 301.55 - 942 K)

$$C_p^0 = 20.783 + 7.1922 \times 10^{-9} T^2$$

(EQUATION VALID FROM 942 - 1800 K)

REFERENCE 107 35

COMPILED  
5-12-76

COPPER (REFERENCE STATE) FORMULA WEIGHT 63.546

Cu: Face-centered cubic crystals 298.15 to melting point 1356 K. Liquid 1356 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	33.15	33.15	24.45	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	6.357	40.48	34.12	25.43	.000	.000	.000
500	10.246	46.24	35.99	26.15	.000	.000	.000
600	12.948	51.06	38.11	26.74	.000	.000	.000
700	14.957	55.22	40.26	27.25	.000	.000	.000
800	16.522	58.89	42.37	27.71	.000	.000	.000
900	17.790	62.18	44.39	28.14	.000	.000	.000
1000	18.845	65.16	46.32	28.53	.000	.000	.000
1100	19.743	67.90	48.16	28.92	.000	.000	.000
1200	20.522	70.43	49.91	29.28	.000	.000	.000
1300	21.211	72.79	51.58	29.64	.000	.000	.000
1356.55	21.695	74.13	52.43	29.85	.000	.000	.000
1356.55	31.318	83.75	52.43	32.64	.000	.000	.000
1400	31.320	84.70	53.38	32.64	.000	.000	.000
1500	31.324	86.87	55.55	32.64	.000	.000	.000
1600	31.327	88.88	57.55	32.64	.000	.000	.000
1700	31.331	90.76	59.43	32.64	.000	.000	.000
1800	31.333	92.56	61.23	32.64	.000	.000	.000

MELTING POINT	1356.55 K	BOILING POINT	2836 K
ENTHALPY OF MELTING	13.054 kJ	ENTHALPY OF VAPORIZATION	300.340 kJ
$H_{298}^0 - H_0^0$	5.004 kJ	MOLAR VOLUME	0.7113 J/bar 7.113 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 29.764 + 1.6124 \times 10^{-3} T + 3.4110 \times 10^{-7} T^2 - 1.0067 \times 10^2 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1356.55 K)

REFERENCE 107

35

COMPILED  
5-12-76

DYSPROSIUM (REFERENCE STATE)

FORMULA WEIGHT 162.500

Dy: Alpha crystals (hexagonal close packed) 298.15 to 1657 K. Beta crystals (body-centered cubic) 1657 to melting point 1682 K. Liquid 1682 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	74.89	74.89	28.11	0.000	0.000	0.000
UNCERTAINTY		0.84	0.84				
400	7.160	83.15	75.99	28.14	.000	.000	.000
500	11.358	89.44	78.08	28.17	.000	.000	.000
600	14.173	94.58	80.41	28.35	.000	.000	.000
700	16.224	98.98	82.76	28.77	.000	.000	.000
800	17.835	102.87	85.03	29.49	.000	.000	.000
900	19.186	106.40	87.21	30.54	.000	.000	.000
1000	20.387	109.68	89.29	31.93	.000	.000	.000
1100	21.514	112.81	91.30	33.68	.000	.000	.000
1200	22.613	115.83	93.22	35.80	.000	.000	.000
1300	23.721	118.79	95.07	38.30	.000	.000	.000
1400	24.863	121.73	96.87	41.18	.000	.000	.000
1500	26.057	124.68	98.62	44.44	.000	.000	.000
1600	27.318	127.66	100.34	48.09	.000	.000	.000
1657	28.076	129.41	101.34	50.17	.000	.000	.000
1657	30.588	131.92	101.34	28.03	.000	.000	.000
1682	30.549	132.34	101.76	28.03	.000	.000	.000
1682	37.124	138.91	101.76	49.92	.000	.000	.000
1700	37.257	139.41	102.15	49.91	.000	.000	.000
1800	37.960	142.29	104.33	49.91	.000	.000	.000

MELTING POINT	1682 K	BOILING POINT	2835 K
ENTHALPY OF MELTING	11.058 kJ	ENTHALPY OF VAPORIZATION	230.095 kJ
$H_{298}^0 - H_0^0$	8.866 kJ	MOLAR VOLUME	1.9010 J/bar 19.010 $\text{cm}^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 45.108 - 2.7561 \times 10^{-2} T + 2.0181 \times 10^{-5} T^2 - 1.8339 \times 10^{-8} T^{0.5}$$

(EQUATION VALID FROM 298 - 1657 K)

REFERENCE 107 107

COMPILED  
4-27-76



ERBIUM (REFERENCE STATE)

FORMULA WEIGHT 167.260

Er: Hexagonal close packed crystals 298.15 to melting point 1795 K. Liquid  
1795 to boiling point 3136 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	73.18	73.18	28.05	0.000	0.000	0.000
UNCERTAINTY		0.15	0.15				
400	7.190	81.48	74.29	28.41	.000	.000	.000
500	11.468	87.85	76.38	28.76	.000	.000	.000
600	14.385	93.13	78.74	29.19	.000	.000	.000
700	16.539	97.67	81.13	29.74	.000	.000	.000
800	18.229	101.69	83.46	30.40	.000	.000	.000
900	19.623	105.31	85.69	31.18	.000	.000	.000
1000	20.823	108.64	87.82	32.08	.000	.000	.000
1100	21.892	111.75	89.86	33.09	.000	.000	.000
1200	22.872	114.67	91.80	34.22	.000	.000	.000
1300	23.791	117.46	93.67	35.46	.000	.000	.000
1400	24.671	120.14	95.47	36.80	.000	.000	.000
1500	25.529	122.72	97.19	38.26	.000	.000	.000
1600	26.372	125.24	98.87	39.83	.000	.000	.000
1700	27.213	127.71	100.50	41.50	.000	.000	.000
1795	28.011	130.04	102.05	43.22	.000	.000	.000
1795	39.099	141.13	102.05	38.70	.000	.000	.000
1800	39.099	141.20	102.10	38.70	.000	.000	.000

MELTING POINT	1795	K	BOILING POINT	3136	K
ENTHALPY OF MELTING	19.903	kJ	ENTHALPY OF VAPORIZATION	261.350	kJ
$H_{298}^0 - H_0^0$	7.392	kJ	MOLAR VOLUME		J/bar

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 24.717 + 5.2252 \times 10^{-6} T^2 + 71.155 T^{-0.5} - 1.1163 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1795 K)

REFERENCE 107 107

COMPILED  
4-15-76

## EUROPIUM (REFERENCE STATE)

FORMULA WEIGHT 151.960

Eu: Body-centered cubic crystals 298.15 to melting point 1090 K. Liquid  
1090 to boiling point 1870 K.

FORMATION FROM THE ELEMENTS  
GIBBS

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	80.79	80.79	27.12	0.000	0.000	0.000
UNCERTAINTY		0.16	0.16				
400	6.990	88.85	81.86	27.96	.000	.000	.000
500	11.334	95.25	83.92	29.55	.000	.000	.000
600	14.457	100.74	86.28	30.30	.000	.000	.000
700	16.800	105.49	88.69	31.44	.000	.000	.000
800	18.721	109.79	91.07	33.02	.000	.000	.000
900	20.429	113.80	93.37	35.26	.000	.000	.000
1000	22.048	117.65	95.60	38.07	.000	.000	.000
1090	23.476	121.06	97.58	40.92	.000	.000	.000
1090	31.928	129.51	97.58	38.12	.000	.000	.000
1100	31.985	129.84	97.86	38.12	.000	.000	.000
1200	32.496	133.16	100.66	38.12	.000	.000	.000
1300	32.928	136.21	103.28	38.12	.000	.000	.000
1400	33.299	139.04	105.74	38.12	.000	.000	.000
1500	33.620	141.67	108.05	38.12	.000	.000	.000
1600	33.901	144.13	110.23	38.12	.000	.000	.000
1700	34.149	146.44	112.29	38.12	.000	.000	.000
1800	34.369	148.62	114.25	38.12	.000	.000	.000

MELTING POINT	1090 K	BOILING POINT	1870 K
ENTHALPY OF MELTING	9.213 kJ	ENTHALPY OF VAPORIZATION	143.500 kJ
$H_{298}^0 - H_0^0$		MOLAR VOLUME	2.8970 J/bar 28.970 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 3.1897 \times 10^{-2} T + 3.0408 \times 10^{-2} T^{-0.5}$$

(EQUATION VALID FROM 298 - 503.15 K)

$$C_P^0 = -5.3514 \times 10^{-2} + 0.28764 T - 5.7795 \times 10^{-5} T^2 + 1.1488 \times 10^{-8} T^{-0.5}$$

$$-1.9919 \times 10^{-7} T^{-2}$$

EQUATION VALID FROM 503.15 - 1090 K)

REFERENCE 107 107

COMPILED  
4-15-76

FLUORINE (REFERENCE STATE)

FORMULA WEIGHT 37.997

F<sub>2</sub>: Ideal diatomic gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	202.79	202.79	31.32	0.000	0.000	0.000
UNCERTAINTY		0.04	0.04				
400	8.210	212.25	204.04	33.07	.000	.000	.000
500	13.312	219.77	206.46	34.32	.000	.000	.000
600	16.893	226.11	209.22	35.24	.000	.000	.000
700	19.567	231.60	212.03	35.93	.000	.000	.000
800	21.647	236.44	214.79	36.47	.000	.000	.000
900	23.319	240.76	217.44	36.90	.000	.000	.000
1000	24.695	244.66	219.97	37.24	.000	.000	.000
1100	25.849	248.23	222.38	37.53	.000	.000	.000
1200	26.832	251.50	224.67	37.78	.000	.000	.000
1300	27.683	254.54	226.86	37.99	.000	.000	.000
1400	28.426	257.36	228.93	38.19	.000	.000	.000
1500	29.083	260.00	230.92	38.38	.000	.000	.000
1600	29.670	262.48	232.81	38.55	.000	.000	.000
1700	30.198	264.82	234.62	38.73	.000	.000	.000
1800	30.676	267.04	236.36	38.90	.000	.000	.000

MELTING POINT	53.48 K	BOILING POINT	84.95 K
ENTHALPY OF MELTING	0.510 kJ	ENTHALPY OF VAPORIZATION	6.535 kJ
$H_{298}^0 - H_0^0$	8.825 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 53.265 - 5.1095 \times 10^{-3} T + 1.2226 \times 10^{-6} T^2 - 3.8948 \times 10^2 T^{-0.5} + 1.8029 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 35

COMPILED  
3-11-76

## IRON (REFERENCE STATE)

FORMULA WEIGHT 55.847

Fe: Alpha crystals (body-centered cubic) 298.15 to 1184 K. Curie point 1042 K. Gamma crystals (face-centered cubic) 1184 to 1665 K. Delta crystals (body-centered cubic) 1665 to melting point 1809 K. Liquid from 1809 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		Log K <sub>f</sub>
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	
298.15	0.000	27.28	27.28	24.98	0.000	0.000	0.000
UNCERTAINTY		0.13	0.13				
400	6.642	34.94	28.29	27.36	.000	.000	.000
500	10.962	41.25	30.29	29.71	.000	.000	.000
600	14.225	46.82	32.59	32.05	.000	.000	.000
700	16.916	51.88	34.97	34.60	.000	.000	.000
800	19.351	56.73	37.38	37.95	.000	.000	.000
900	21.757	61.59	39.83	43.10	.000	.000	.000
1000	24.435	66.69	42.26	54.43	.000	.000	.000
1042	25.345	68.84	43.50	83.68	.000	.000	.000
1042	26.265	69.76	43.50	54.25	.000	.000	.000
1100	27.462	72.22	44.75	46.40	.000	.000	.000
1184	28.376	75.19	46.81	41.42	.000	.000	.000
1184	29.136	75.95	46.81	33.89	.000	.000	.000
1200	29.253	76.44	47.19	34.02	.000	.000	.000
1300	29.642	79.16	49.52	34.85	.000	.000	.000
1400	30.035	81.76	51.72	35.69	.000	.000	.000
1500	30.404	84.22	53.82	36.53	.000	.000	.000
1600	30.779	86.57	55.79	37.36	.000	.000	.000
1665	31.036	88.09	57.06	37.91	.000	.000	.000
1665	31.646	88.70	57.06	41.13	.000	.000	.000
1700	31.848	89.54	57.69	41.46	.000	.000	.000
1800	32.379	91.92	59.54	42.47	.000	.000	.000

MELTING POINT	1809 K	BOILING POINT	3135 K
ENTHALPY OF MELTING	13.807 kJ	ENTHALPY OF VAPORIZATION	349.590 kJ
$H_{298}^0 - H_0^0$	4.489 kJ	MOLAR VOLUME	0.7092 J/bar 7.092 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE	107	107	COMPILED 6-13-66
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GALLIUM (REFERENCE STATE)

FORMULA WEIGHT 69.720

Ga: Orthorhombic crystals 298.15 to melting point 302.9 K. Liquid 302.9 to boiling point 2478 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	40.83	40.83	26.22	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
302.9	0.428	41.25	40.83	27.36	.000	.000	.000
302.9	18.883	59.70	40.83	28.49	.000	.000	.000
400	21.000	67.39	46.39	27.23	.000	.000	.000
500	22.192	73.41	51.22	26.78	.000	.000	.000
600	22.943	78.28	55.34	26.63	.000	.000	.000
700	23.464	82.38	58.92	26.57	.000	.000	.000
800	23.852	85.93	62.08	26.57	.000	.000	.000
900	24.156	89.06	64.90	26.57	.000	.000	.000
1000	24.398	91.86	67.46	26.57	.000	.000	.000
1100	24.597	94.39	69.79	26.57	.000	.000	.000
1200	24.763	96.71	71.95	26.57	.000	.000	.000
1300	24.905	98.84	73.94	26.57	.000	.000	.000
1400	25.025	100.81	75.78	26.57	.000	.000	.000
1500	25.128	102.64	77.51	26.57	.000	.000	.000
1600	25.217	104.35	79.13	26.57	.000	.000	.000
1700	25.295	105.96	80.67	26.57	.000	.000	.000
1800	25.362	107.48	82.12	26.57	.000	.000	.000

MELTING POINT	302.90 K	BOILING POINT	2478 K
ENTHALPY OF MELTING	5,590 kJ	ENTHALPY OF VAPORIZATION	258,720 kJ
$H_{298}^0 - H_0^0$	5,573 kJ	MOLAR VOLUME	1.1790 J/bar 11.790 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 31.155 - 1.0116 \times 10^{-3} T - 1.2666 \times 10^2 T^{-0.5} + 4.4944 \times 10^5 T^{-2}$$

EQUATION VALID FROM 302.90 - 700 K)

REFERENCE 107 107 COMPILED 4-13-76

## GADOLINIUM (REFERENCE STATE)

FORMULA WEIGHT 157.250

Gd: Alpha crystals (hexagonal close packed) 298.15 to 1533 K. Beta crystals (body-centered cubic) 1533 to melting point 1585 K. Liquid 1585 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	68.45	68.45	26.15	0.000	0.000	0.000
UNCERTAINTY		1.25	1.25				
400	7.877	77.53	69.65	27.15	.000	.000	.000
500	11.932	83.80	71.87	26.82	.000	.000	.000
600	14.728	89.12	74.39	26.69	.000	.000	.000
700	16.844	93.68	76.84	26.57	.000	.000	.000
800	18.540	97.74	79.20	26.57	.000	.000	.000
900	19.953	101.42	81.47	26.57	.000	.000	.000
1000	21.167	104.77	83.60	26.57	.000	.000	.000
1100	22.236	107.95	85.71	26.57	.000	.000	.000
1200	23.214	110.88	87.66	26.57	.000	.000	.000
1300	24.125	113.68	89.55	26.57	.000	.000	.000
1400	24.994	116.40	91.41	26.57	.000	.000	.000
1500	25.829	118.99	93.16	26.57	.000	.000	.000
1533	26.106	119.33	93.22	38.70	.000	.000	.000
1533	28.658	121.88	93.22	28.28	.000	.000	.000
1585	28.654	122.80	94.14	28.28	.000	.000	.000
1585	34.998	129.16	94.14	37.15	.000	.000	.000
1600	35.017	130.00	94.98	37.15	.000	.000	.000
1700	35.143	132.26	97.11	37.15	.000	.000	.000
1800	35.255	134.39	99.13	37.15	.000	.000	.000

MELTING POINT	1585	K	BOILING POINT	3539	K
ENTHALPY OF MELTING	10.054	kJ	ENTHALPY OF VAPORIZATION	359.380	kJ
$H_{298}^0 - H_0^0$	9.079	kJ	MOLAR VOLUME	1.9890	J/bar
				19.890	cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE	107	107	COMPILED
			5-15-73

GERMANIUM (REFERENCE STATE)

FORMULA WEIGHT 72.590

Ge: Face-centered cubic crystals (diamond structure) 298.15 to 1210.4 K.

Liquid 1210.4 to boiling point 3107 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	31.09	31.09	23.39	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.100	38.12	32.02	24.38	.000	.000	.000
500	9.810	43.62	33.81	24.89	.000	.000	.000
600	12.355	48.19	35.83	25.25	.000	.000	.000
700	14.223	52.11	37.89	25.60	.000	.000	.000
800	15.670	55.56	39.89	26.01	.000	.000	.000
900	16.844	58.65	41.81	26.50	.000	.000	.000
1000	17.839	61.47	43.63	27.11	.000	.000	.000
1100	18.715	64.09	45.38	27.85	.000	.000	.000
1200	19.511	66.55	47.04	28.73	.000	.000	.000
1210.4	19.595	66.93	47.33	28.83	.000	.000	.000
1210.4	50.118	97.45	47.33	27.61	.000	.000	.000
1300	48.567	99.29	50.72	27.61	.000	.000	.000
1400	47.070	101.34	54.27	27.61	.000	.000	.000
1500	45.773	103.25	57.48	27.61	.000	.000	.000
1600	44.638	105.03	60.39	27.61	.000	.000	.000
1700	43.637	106.70	63.06	27.61	.000	.000	.000
1800	42.747	108.28	65.53	27.61	.000	.000	.000

MELTING POINT	1210.4 K	BOILING POINT	3107 K
ENTHALPY OF MELTING	36.945 kJ	ENTHALPY OF VAPORIZATION	330.915 kJ
$H_{298}^0 - H_0^0$	4.627 kJ	MOLAR VOLUME	1.3630 J/bar 13.630 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 37.798 - 1.3888 \times 10^{-2} T + 8.8359 \times 10^{-6} T^2 - 1.7583 \times 10^{-9} T^3 - 7.6972 \times 10^{-12} T^4$$

(EQUATION VALID FROM 298 - 1210.4 K)

REFERENCE 107 107

COMPILED  
4-12-76

HYDROGEN (REFERENCE STATE) FORMULA WEIGHT 2.016

H<sub>2</sub>: Ideal diatomic gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	130.68	130.68	28.84	0.000	0.000	0.000
UNCERTAINTY		0.04	0.04				
400	7.407	139.23	131.82	29.22	.000	.000	.000
500	11.774	145.75	133.98	29.25	.000	.000	.000
600	14.690	151.09	136.40	29.29	.000	.000	.000
700	16.783	155.61	138.83	29.42	.000	.000	.000
800	18.375	159.55	141.17	29.62	.000	.000	.000
900	19.639	163.06	143.42	29.90	.000	.000	.000
1000	20.681	166.22	145.54	30.22	.000	.000	.000
1100	21.564	169.12	147.56	30.58	.000	.000	.000
1200	22.332	171.80	149.47	30.98	.000	.000	.000
1300	23.012	174.29	151.28	31.39	.000	.000	.000
1400	23.626	176.63	153.00	31.81	.000	.000	.000
1500	24.185	178.84	154.65	32.24	.000	.000	.000
1600	24.702	180.94	156.24	32.67	.000	.000	.000
1700	25.184	182.93	157.75	33.10	.000	.000	.000
1800	25.635	184.83	159.19	33.52	.000	.000	.000

MELTING POINT	13.80 K	BOILING POINT	20.27 K
ENTHALPY OF MELTING	0.117 kJ	ENTHALPY OF VAPORIZATION	0.904 kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	8.468 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

HEAT CAPACITY EQUATION

$$C_P^0 = 7.4424 + 1.1707 \times 10^{-2} T - 1.3899 \times 10^{-6} T^2 + 4.1017 \times 10^{-9} T^3 - 5.1041 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 35 COMPILED  
3-11-76



HELIUM (REFERENCE STATE) FORMULA WEIGHT 4.003

He: Ideal gas 298.15 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	126.15	126.15	20.79	0.000	0.000	0.000
UNCERTAINTY		0.01	0.01				
400	5.292	132.26	126.97	20.79	.000	.000	.000
500	8.392	136.90	128.51	20.79	.000	.000	.000
600	10.457	140.69	130.23	20.79	.000	.000	.000
700	11.933	143.89	131.96	20.79	.000	.000	.000
800	13.040	146.67	133.63	20.79	.000	.000	.000
900	13.900	149.11	135.21	20.79	.000	.000	.000
1000	14.589	151.30	136.71	20.79	.000	.000	.000
1100	15.152	153.29	138.14	20.79	.000	.000	.000
1200	15.622	155.09	139.47	20.79	.000	.000	.000
1300	16.019	156.76	140.74	20.79	.000	.000	.000
1400	16.359	158.30	141.94	20.79	.000	.000	.000
1500	16.655	159.73	143.08	20.79	.000	.000	.000
1600	16.912	161.07	144.16	20.79	.000	.000	.000
1700	17.141	162.33	145.19	20.79	.000	.000	.000
1800	17.343	163.52	146.18	20.79	.000	.000	.000

MELTING POINT	K	BOILING POINT	4.21 K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	6.197 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

REFERENCE 107 35 COMPILED 3-11-76

HAFNIUM (REFERENCE STATE) FORMULA WEIGHT 178.490

Hf: Alpha crystals (hexagonal close packed) 298.15 to 2013 K. Beta crystals  
(body-centered cubic) 2103 to melting point 2500 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	43.56	43.56	25.64	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.645	51.22	44.57	26.52	.000	.000	.000
500	10.698	57.22	46.52	27.30	.000	.000	.000
600	13.528	62.27	48.74	28.06	.000	.000	.000
700	15.657	66.65	50.99	28.81	.000	.000	.000
800	17.349	70.55	53.20	29.56	.000	.000	.000
900	18.747	74.07	55.32	30.31	.000	.000	.000
1000	19.941	77.30	57.36	31.07	.000	.000	.000
1100	20.987	80.30	59.31	31.83	.000	.000	.000
1200	21.922	83.10	61.18	32.59	.000	.000	.000
1300	22.772	85.74	62.97	33.35	.000	.000	.000
1400	23.554	88.24	64.69	34.12	.000	.000	.000
1500	24.284	90.62	66.34	34.88	.000	.000	.000
1600	24.971	92.90	67.93	35.65	.000	.000	.000
1700	25.621	95.08	69.46	36.42	.000	.000	.000
1800	26.243	97.18	70.94	37.19	.000	.000	.000

MELTING POINT	2500 K	BOILING POINT	4876 K
ENTHALPY OF MELTING	24.058 kJ	ENTHALPY OF VAPORIZATION	575.141 kJ
$H_{298}^0 - H_0^0$	5.845 kJ	MOLAR VOLUME	13.479 J/bar 13.479 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 22.465 + 7.8597 \times 10^{-3} T + 25.261 T^{-0.5} - 5.5918 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76

MERCURY (REFERENCE STATE) FORMULA WEIGHT 200.590

Hg: Liquid 298.15 to boiling point 629.0 K. Ideal monatomic gas 629.0 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS						
				GIBBS			
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	75.90	75.90	27.96	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	7.042	84.03	76.99	27.41	.000	.000	.000
500	11.088	90.12	79.03	27.17	.000	.000	.000
600	13.763	95.07	81.31	27.14	.000	.000	.000
629.0	14.380	96.35	81.97	27.17	.000	.000	.000
629.0	108.520	190.49	81.97	20.79	.000	.000	.000
700	99.622	192.71	93.09	20.79	.000	.000	.000
800	89.768	195.48	105.71	20.79	.000	.000	.000
900	82.104	197.93	115.83	20.79	.000	.000	.000
1000	75.972	200.12	124.15	20.79	.000	.000	.000
1100	70.956	202.10	141.14	20.79	.000	.000	.000
1200	66.775	203.91	137.14	20.79	.000	.000	.000
1300	63.238	205.58	142.34	20.79	.000	.000	.000
1400	60.206	207.12	146.91	20.79	.000	.000	.000
1500	57.579	208.55	150.97	20.79	.000	.000	.000
1610	55.279	209.89	154.61	20.79	.000	.000	.000
1700	53.250	211.15	157.90	20.79	.000	.000	.000
1800	51.447	212.34	160.89	20.79	.000	.000	.000

MELTING POINT	234.29 K	BOILING POINT	629.0 K
ENTHALPY OF MELTING	2.297 kJ	ENTHALPY OF VAPORIZATION	59.214 kJ
$H_{298}^0 - H_0^0$	9.343 kJ	MOLAR VOLUME	1.4822 J/bar 14.822 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 16.817 + 3.6233 \times 10^{-3} T + 2.1681 \times 10^{-6} T^2 + 1.8595 \times 10^{-9} T^{-0.5} - 7.9563 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 629 K)

REFERENCE 107 107 COMPILED 4-10-76

HOLMIUM (REFERENCE STATE)

FORMULA WEIGHT 164.930

Ho: Alpha crystals (hexagonal close packed) 298.15 to 1701 K. Beta crystals (body-centered cubic) 1701 to melting point 1743 K. Liquid 1743 to boiling point 2968 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	75.02	75.02	27.11	0.000	0.000	0.000
UNCERTAINTY		1.67	1.67				
400	7.037	83.14	76.10	27.91	.000	.000	.000
500	11.224	89.38	78.16	28.00	.000	.000	.000
600	14.028	94.49	80.46	28.14	.000	.000	.000
700	16.070	98.86	82.79	28.55	.000	.000	.000
800	17.674	102.71	85.04	29.30	.000	.000	.000
900	19.023	106.23	87.21	30.41	.000	.000	.000
1000	20.232	109.50	89.27	31.88	.000	.000	.000
1100	21.371	112.62	91.25	33.71	.000	.000	.000
1200	22.488	115.65	93.16	35.90	.000	.000	.000
1300	23.616	118.62	95.00	38.45	.000	.000	.000
1400	24.777	121.57	96.79	41.36	.000	.000	.000
1500	25.989	124.54	98.55	44.61	.000	.000	.000
1600	27.264	127.53	100.27	48.22	.000	.000	.000
1700	28.611	130.57	101.96	52.17	.000	.000	.000
1701	28.634	130.58	101.96	52.13	.000	.000	.000
1701	31.391	133.34	101.96	28.03	.000	.000	.000
1743	31.309	134.06	102.74	28.03	.000	.000	.000
1743	38.297	141.04	102.74	43.93	.000	.000	.000
1800	38.476	142.45	103.97	43.93	.000	.000	.000

MELTING POINT	1743 K	BOILING POINT	2968 K
ENTHALPY OF MELTING	12.180 kJ	ENTHALPY OF VAPORIZATION	240.980 kJ
$H_{298}^0 - H_0^0$	7.996 kJ	MOLAR VOLUME	1.8740 J/bar 18.740 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_p^0 = 19.256 - 1.3024 \times 10^{-2} T + 1.6534 \times 10^{-5} T^2 + 3.0961 \times 10^{-8} T^3 - 6.8162 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1701 K)

REFERENCE 107 107

COMPILED  
4-27-76

IODINE ( REFERENCE STATE )

FORMULA WEIGHT 253.809

I<sub>2</sub>: Crystals 298.15 to melting point 386.75 K. Liquid 386.75 to boiling point 458 K. Ideal diatomic gas 458 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	116.25	116.25	54.44	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
386.75	13.220	131.21	117.99	61.67	.000	.000	.000
386.75	53.681	171.67	117.99	82.84	.000	.000	.000
400	54.642	174.49	119.85	82.01	.000	.000	.000
458	58.108	185.58	127.47	82.01	.000	.000	.000
458	149.158	276.63	127.47	37.38	.000	.000	.000
500	139.771	279.91	140.14	37.45	.000	.000	.000
600	122.729	286.76	164.03	37.60	.000	.000	.000
700	110.598	292.56	181.98	37.71	.000	.000	.000
800	101.473	297.60	196.13	37.81	.000	.000	.000
900	94.405	302.06	207.60	37.90	.000	.000	.000
1000	88.759	330.30	217.30	37.99	.000	.000	.000
1100	84.147	309.68	225.53	38.07	.000	.000	.000
1200	80.310	313.00	232.69	38.15	.000	.000	.000
1300	77.070	316.06	238.99	38.23	.000	.000	.000
1400	74.299	318.89	244.59	38.31	.000	.000	.000
1500	71.902	321.54	249.64	38.39	.000	.000	.000
1600	69.810	324.02	254.21	38.47	.000	.000	.000
1700	67.969	326.35	258.38	38.56	.000	.000	.000
1800	66.337	328.56	262.22	38.64	.000	.000	.000

MELTING POINT	386.75 K	BOILING POINT	458 K
ENTHALPY OF MELTING	15.648 kJ	ENTHALPY OF VAPORIZATION	41.700 kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	13.196 kJ	MOLAR VOLUME	5.1290 J/bar 51.290 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 37.872 + 3.4318 \times 10^{-4} T + 1.2026 \times 10^{-7} T^2 - 9.5174 T^{-0.5} - 4.8784 \times 10^4 T^{-2}$$

EQUATION VALID FROM 458 - 1800 K)

REFERENCE 107 35 COMPILED 5-24-76

INDIUM (REFERENCE STATE)

FORMULA WEIGHT 114.820

In: Tetragonal crystals 298.15 to melting point 429.76 K. Liquid 429.76 to boiling point 2346 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	57.84	57.84	26.73	0.000	0.000	0.000
UNCERTAINTY		0.84	0.84				
400	7.030	65.94	58.91	28.97	.000	.000	.000
429.76	8.632	68.78	60.15	30.33	.000	.000	.000
429.76	16.227	76.38	60.15	29.47	.000	.000	.000
500	18.076	80.14	62.06	29.44	.000	.000	.000
600	19.962	85.50	65.54	29.33	.000	.000	.000
700	21.293	90.02	68.73	29.23	.000	.000	.000
800	22.280	93.91	71.63	29.15	.000	.000	.000
900	23.040	97.34	74.30	29.10	.000	.000	.000
1000	23.645	100.41	76.76	29.07	.000	.000	.000
1100	24.137	103.18	79.04	29.06	.000	.000	.000
1200	24.548	105.71	81.16	29.06	.000	.000	.000
1300	24.895	108.03	83.13	29.07	.000	.000	.000
1400	25.194	110.19	85.00	29.08	.000	.000	.000
1500	25.453	112.20	86.75	29.09	.000	.000	.000
1600	25.681	114.07	88.39	29.10	.000	.000	.000
1700	25.882	115.84	89.96	29.10	.000	.000	.000
1800	26.061	117.50	91.44	29.10	.000	.000	.000

MELTING POINT	429.76 K	BOILING POINT	2346 K
ENTHALPY OF MELTING	3.264 kJ	ENTHALPY OF VAPORIZATION	231.450 kJ
$H_{298}^0 - H_0^0$	6.602 kJ	MOLAR VOLUME	1.5753 J/bar 15.753 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATIONS

$$C_p^0 = 2.9024 \times 10^2 - 0.48417 T + 4.5808 \times 10^{-4} T^2 - 2.9213 \times 10^{-3} T^{-0.5} + 8.2737 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 429.76 K)

$$C_p^0 = 16.334 + 5.4841 \times 10^{-3} T - 1.0873 \times 10^{-6} T^2 + 2.7803 \times 10^2 T^{-0.5} - 4.4951 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 429.76 - 1800 K)

REFERENCE 107 107

COMPILED  
5-06-76

IRIDIUM (REFERENCE STATE)

FORMULA WEIGHT 192.220

Ir: Face-centered cubic crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	35.48	35.48	24.93	0.000	0.000	0.000
UNCERTAINTY		0.17	0.17				
400	6.427	42.89	36.46	25.52	.000	.000	.000
500	10.296	48.64	38.34	26.03	.000	.000	.000
600	12.963	53.44	40.48	26.59	.000	.000	.000
700	14.954	57.58	42.63	27.22	.000	.000	.000
800	16.530	61.26	44.73	27.90	.000	.000	.000
900	17.832	64.59	46.76	28.61	.000	.000	.000
1000	18.947	67.64	48.69	29.35	.000	.000	.000
1100	19.926	70.47	50.54	30.10	.000	.000	.000
1200	20.807	73.12	52.31	30.86	.000	.000	.000
1300	21.609	75.62	54.01	31.62	.000	.000	.000
1400	22.351	77.99	55.64	32.38	.000	.000	.000
1500	23.044	80.25	57.21	33.12	.000	.000	.000
1600	23.697	82.42	58.72	33.86	.000	.000	.000
1700	24.316	84.49	60.17	34.59	.000	.000	.000
1800	24.907	86.49	61.58	35.30	.000	.000	.000

MELTING POINT	2716 K	BOILING POINT	4701 K
ENTHALPY OF MELTING	26.137 kJ	ENTHALPY OF VAPORIZATION	604.075 kJ
$H_{298}^0 - H_0^0$	5.268 kJ	MOLAR VOLUME	0.8519 J/bar 8.519 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

HEAT CAPACITY EQUATION

$$C_P^0 = 10.073 + 1.3472 \times 10^{-2} T - 1.3835 \times 10^{-6} T^2 + 2.3469 \times 10^{-2} T^{-0.5} - 2.3329 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107 COMPILED 4-17-76

POTASSIUM (REFERENCE STATE)

FORMULA WEIGHT 39.098

K: Body-centered cubic crystals 298.15 to melting point 336.4 K. Liquid  
336.4 to boiling point 1030 K. Ideal monatomic gas 1030 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	64.68	64.68	29.55	0.000	0.000	0.000
UNCERTAINTY		0.20	0.20				
336.35	3.483	68.38	64.92	32.25	.000	.000	.000
336.35	10.424	75.32	64.92	32.14	.000	.000	.000
400	13.830	80.83	67.00	31.55	.000	.000	.000
500	17.284	87.78	70.50	30.69	.000	.000	.000
600	19.465	93.31	73.85	30.10	.000	.000	.000
700	20.961	97.93	76.97	29.82	.000	.000	.000
800	22.065	101.91	79.85	29.81	.000	.000	.000
900	22.934	105.43	82.50	30.00	.000	.000	.000
1000	23.658	108.61	84.95	30.36	.000	.000	.000
1030	23.855	109.51	85.65	30.51	.000	.000	.000
1030	101.445	187.10	85.65	20.79	.000	.000	.000
1100	96.312	187.47	91.16	20.79	.000	.000	.000
1200	90.019	189.28	99.26	20.79	.000	.000	.000
1300	84.694	190.94	106.25	20.79	.000	.000	.000
1400	80.129	192.49	112.36	20.80	.000	.000	.000
1500	76.173	193.92	117.75	20.80	.000	.000	.000
1600	72.712	195.26	122.55	20.81	.000	.000	.000
1700	69.657	196.53	126.87	20.82	.000	.000	.000
1800	66.943	197.72	130.78	20.82	.000	.000	.000

MELTING POINT	336.35 K	BOILING POINT	1030 K
ENTHALPY OF MELTING	2.334 kJ	ENTHALPY OF VAPORIZATION	79.918 kJ
$H_{298}^0 - H_0^0$	7.088 kJ	MOLAR VOLUME	4.5360 J/bar 45.360 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATIONS

$$C_P^0 = -8.9054 + 1.5236 \times 10^{-2} T + 7.8457 \times 10^{-5} T^2 - 7.7864 \times 10^{-8} T^3$$

(EQUATION VALID FROM 336.4 - 1030 K)

$$C_P^0 = 20.801 - 5.1832 \times 10^{-5} T + 3.5737 \times 10^{-8} T^2$$

(EQUATION VALID FROM 1030 - 1800 K)

REFERENCE 107 35

COMPILED  
5-03-76



KRYPTON ( REFERENCE STATE )

FORMULA WEIGHT 83.800

Kr: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	164.08	164.08	20.79	0.000	0.000	0.000
UNCERTAINTY		0.02	0.02				
400	5.292	170.19	164.90	20.79	.000	.000	.000
500	8.392	174.83	166.44	20.79	.000	.000	.000
600	10.457	178.62	168.16	20.79	.000	.000	.000
700	11.933	181.82	169.89	20.79	.000	.000	.000
800	13.040	184.60	171.56	20.79	.000	.000	.000
900	13.900	187.04	173.14	20.79	.000	.000	.000
1000	14.589	189.23	174.64	20.79	.000	.000	.000
1100	15.152	191.22	176.07	20.79	.000	.000	.000
1200	15.622	193.02	177.40	20.79	.000	.000	.000
1300	16.019	194.69	178.67	20.79	.000	.000	.000
1400	16.359	196.23	179.87	20.79	.000	.000	.000
1500	16.655	197.66	181.01	20.79	.000	.000	.000
1600	16.912	199.00	182.09	20.79	.000	.000	.000
1700	17.141	200.26	183.12	20.79	.000	.000	.000
1800	17.343	201.45	184.11	20.79	.000	.000	.000

MELTING POINT	115.78 K	BOILING POINT	K
ENTHALPY OF MELTING	1.636 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	6.197 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE	107	35	COMPILED 3-11-76
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LANTHANUM (REFERENCE STATE)

FORMULA WEIGHT 138.906

La: Alpha crystals (hexagonal close packed) 298.15 to 550 K. Beta crystals (face-centered cubic) 550 to 1134 K. Gamma crystals (body-centered cubic) 1134 to melting point 1193 K. Liquid 1193 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	56.90	56.90	27.10	0.000	0.000	0.000
UNCERTAINTY		2.51	2.51				
400	6.950	64.92	57.97	27.40	.000	.000	.000
500	11.056	71.05	59.99	27.58	.000	.000	.000
550	12.560	73.68	61.13	27.72	.000	.000	.000
550	13.221	74.35	61.13	27.19	.000	.000	.000
600	14.412	76.73	62.32	27.79	.000	.000	.000
700	16.409	81.11	64.70	29.00	.000	.000	.000
800	18.061	85.06	67.00	30.28	.000	.000	.000
900	19.489	88.21	68.72	31.63	.000	.000	.000
1000	20.777	92.11	71.33	33.04	.000	.000	.000
1100	21.959	95.33	73.37	34.52	.000	.000	.000
1134	22.340	96.40	74.06	35.02	.000	.000	.000
1134	25.093	99.16	74.06	39.54	.000	.000	.000
1193	25.812	101.17	75.35	39.54	.000	.000	.000
1193	31.006	106.36	75.35	34.31	.000	.000	.000
1200	31.024	106.54	75.52	34.31	.000	.000	.000
1300	31.277	109.29	78.01	34.31	.000	.000	.000
1400	31.494	111.83	80.34	34.31	.000	.000	.000
1500	31.681	114.20	82.52	34.31	.000	.000	.000
1600	31.846	116.41	84.56	34.31	.000	.000	.000
1700	31.991	118.49	86.50	34.31	.000	.000	.000
1800	32.119	120.45	88.33	34.31	.000	.000	.000

MELTING POINT	1193 K	BOILING POINT	3730 K
ENTHALPY OF MELTING	6.197 kJ	ENTHALPY OF VAPORIZATION	413.670 kJ
$H_{298}^0 - H_0^0$	6.665 kJ	MOLAR VOLUME	2.2470 J/bar 22.470 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.6025 \times 10^{-2} T + 4.8183 \times 10^2 T^{-0.5} - 4.9617 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 550 K)

$$C_P^0 = 1.9885 \times 10^{-2} T + 4.4020 \times 10^2 T^{-0.5} - 7.6150 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 550 - 1134 K)

REFERENCE 107 107

COMPILED  
4-30-76

LITHIUM (REFERENCE STATE)

FORMULA WEIGHT 6.940

Li: Crystals 298.15 to melting point 453.69 K. Liquid 453.69 K to boiling point 1618 K. Ideal monatomic gas 1618 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	29.12	29.12	24.76	0.000	0.000	0.000
UNCERTAINTY		0.02	0.02				
400	6.655	36.78	30.12	27.61	.000	.000	.000
453.70	9.262	40.77	31.51	29.38	.000	.000	.000
453.70	15.874	47.38	31.51	30.44	.000	.000	.000
500	17.158	49.89	32.73	30.05	.000	.000	.000
600	19.255	55.31	36.06	29.48	.000	.000	.000
700	20.690	59.83	39.14	29.14	.000	.000	.000
800	21.732	63.71	41.98	28.94	.000	.000	.000
900	22.528	67.11	44.58	28.83	.000	.000	.000
1000	23.155	70.14	46.98	28.78	.000	.000	.000
1100	23.665	72.89	49.22	28.76	.000	.000	.000
1200	24.089	75.39	51.30	28.75	.000	.000	.000
1300	24.447	77.69	53.24	28.74	.000	.000	.000
1400	24.754	79.82	55.07	28.73	.000	.000	.000
1500	25.018	81.80	56.78	28.71	.000	.000	.000
1600	25.247	83.65	58.40	28.67	.000	.000	.000
1618	25.285	83.97	58.68	28.65	.000	.000	.000
1618	115.245	173.93	58.68	20.80	.000	.000	.000
1700	110.757	174.96	64.20	20.81	.000	.000	.000
1800	105.761	176.15	70.39	20.82	.000	.000	.000

MELTING POINT	453.70 K	BOILING POINT	1618 K
ENTHALPY OF MELTING	3.000 kJ	ENTHALPY OF VAPORIZATION	145.554 kJ
$H_{298}^0 - H_0^0$	4.632 kJ	MOLAR VOLUME	1.3017 J/bar 13.017 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = -38.655 + 6.7350 \times 10^{-2} T + 8.5537 \times 10^{-5} T^2 - 5.5142 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 453.70 K)

$$C_P^0 = 11.835 + 9.1183 \times 10^{-3} T - 2.2265 \times 10^{-6} T^2 + 3.1789 \times 10^{-9} T^3$$

EQUATION VALID FROM 453.70 - 1618 K)

REFERENCE 107 35 COMPILED 5-12-76

LUTETIUM (REFERENCE STATE)

FORMULA WEIGHT 174.970

Lu: Hexagonal close packed crystals 298.15 to melting point 1936 K.

TEMP.	FORMATION FROM THE ELEMENTS						Log $K_f$
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	50.96	50.96	26.76	0.000	0.000	0.000
UNCERTAINTY		0.84	0.84				
400	6.830	58.84	52.01	26.86	.000	.000	.000
500	10.844	64.84	54.00	26.96	.000	.000	.000
600	13.550	69.78	56.23	27.23	.000	.000	.000
700	15.536	74.01	58.47	27.71	.000	.000	.000
800	17.097	77.75	60.65	28.38	.000	.000	.000
900	18.398	81.14	62.74	29.24	.000	.000	.000
1000	19.533	84.28	64.75	30.29	.000	.000	.000
1100	20.565	87.22	66.66	31.51	.000	.000	.000
1200	21.533	90.02	68.49	32.90	.000	.000	.000
1300	22.466	92.71	70.24	34.45	.000	.000	.000
1400	23.382	95.33	71.95	36.17	.000	.000	.000
1500	24.296	97.89	73.59	38.04	.000	.000	.000
1600	25.217	100.41	75.19	40.07	.000	.000	.000
1700	26.155	102.90	76.75	42.25	.000	.000	.000
1800	27.113	105.38	78.27	44.58	.000	.000	.000

MELTING POINT	1936	K	BOILING POINT	3668	K
ENTHALPY OF MELTING	18.648	kJ	ENTHALPY OF VAPORIZATION	355.910	kJ
$H_{298}^0 - H_0^0$	6.389	kJ	MOLAR VOLUME	1.7770 J/bar	
				17.770	cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 17.027 + 7.0407 \times 10^{-6} T^2 + 2.0438 \times 10^{-2} T^{-0.5} - 2.4228 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76

MAGNESIUM (REFERENCE STATE)

FORMULA WEIGHT 24.305

Mg: Hexagonal close packed crystals 298.15 to melting point 922 K. Liquid  
 922 to boiling point 1361 K. Ideal monatomic gas 1361 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	32.68	32.68	24.84	0.000	0.000	0.000
UNCERTAINTY		0.13	0.13				
400	6.497	40.17	33.67	26.15	.000	.000	.000
500	10.546	46.13	35.58	27.31	.000	.000	.000
600	13.433	51.21	37.78	28.45	.000	.000	.000
700	15.661	55.68	40.02	29.61	.000	.000	.000
800	17.479	59.71	42.23	30.79	.000	.000	.000
900	19.024	63.41	44.39	32.00	.000	.000	.000
922	19.338	64.41	45.07	32.27	.000	.000	.000
922	29.050	74.12	45.07	32.64	.000	.000	.000
1000	29.329	76.55	47.22	32.64	.000	.000	.000
1100	29.629	79.66	50.03	32.64	.000	.000	.000
1200	29.880	82.50	52.62	32.64	.000	.000	.000
1300	30.092	85.11	55.02	32.64	.000	.000	.000
1361	30.206	86.37	56.37	32.64	.000	.000	.000
1361	123.678	180.20	56.37	20.79	.000	.000	.000
1400	120.959	180.79	59.83	20.79	.000	.000	.000
1500	114.281	182.22	67.94	20.79	.000	.000	.000
1600	108.438	183.57	75.13	20.79	.000	.000	.000
1700	103.282	184.83	81.55	20.79	.000	.000	.000
1800	98.698	186.01	87.31	20.79	.000	.000	.000

MELTING POINT 922 K BOILING POINT 1361 K  
 ENTHALPY OF MELTING 8.954 kJ ENTHALPY OF VAPORIZATION 127.421 kJ  
 $H_{298}^0 - H_0^0$  5.000 kJ MOLAR VOLUME 1.3996 J/bar  
 13.996 cm<sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 16.095 + 1.3795 \times 10^{-2} T + 1.1053 \times 10^{-5} T^2 - 1.5759 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 922 K)

REFERENCE 107 107

COMPILED  
 4-10-76

## MANGANESE (REFERENCE STATE)

FORMULA WEIGHT 54.938

Mn: Alpha crystals 298.15 to 980 K. Beta crystals 980 to 1360 K. Gamma crystals 1360 to 1410 K. Delta crystals 1410 to melting point 1517 K. Liquid 1517 to boiling point 2335 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	32.01	32.01	26.19	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	6.945	40.01	33.07	28.30	.000	.000	.000
500	11.404	46.53	35.13	30.16	.000	.000	.000
600	14.677	52.18	37.50	31.89	.000	.000	.000
700	17.251	57.22	39.97	33.49	.000	.000	.000
800	19.374	61.79	42.42	34.93	.000	.000	.000
900	21.173	65.98	44.81	36.18	.000	.000	.000
980	22.349	69.05	46.70	37.04	.000	.000	.000
980	24.696	71.40	46.70	37.59	.000	.000	.000
1000	24.960	72.12	47.16	37.68	.000	.000	.000
1100	26.136	75.73	49.59	38.11	.000	.000	.000
1200	27.152	79.07	51.92	38.54	.000	.000	.000
1300	28.044	82.17	54.13	38.97	.000	.000	.000
1360	28.516	84.01	55.49	39.15	.000	.000	.000
1360	29.476	84.97	55.49	42.41	.000	.000	.000
1400	30.468	86.75	56.28	43.43	.000	.000	.000
1410	30.561	87.07	56.51	43.51	.000	.000	.000
1410	31.893	88.41	56.51	45.23	.000	.000	.000
1500	32.716	91.21	58.49	45.97	.000	.000	.000
1517	32.865	91.86	59.00	46.11	.000	.000	.000
1517	40.814	99.81	59.00	46.02	.000	.000	.000
1600	41.084	102.13	61.05	46.02	.000	.000	.000
1700	41.375	104.92	63.55	46.02	.000	.000	.000
1800	41.633	107.55	65.92	46.02	.000	.000	.000

MELTING POINT	1517 K	BOILING POINT	2335 K
ENTHALPY OF MELTING	12.058 kJ	ENTHALPY OF VAPORIZATION	226.065 kJ
$H_{298}^0 - H_0^0$	4.996 kJ	MOLAR VOLUME	0.7354 J/bar 7.354 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATIONS

$$C_p^0 = 4.1345 \times 10^{-2} T - 1.3745 \times 10^{-5} T^2 + 3.1329 \times 10^2 T^{-0.5} - 2.7217 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 980 K)

$$C_p^0 = 33.387 + 4.2936 \times 10^{-3} T$$

(EQUATION VALID FROM 980 - 1360 K)

REFERENCE 107 107

COMPILED  
5-12-76

MOLYBDENUM (REFERENCE STATE)

FORMULA WEIGHT 95.940

Mo: Body-centered cubic crystals 298.15 to melting point 2890 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15 UNCERTAINTY	0.000 0.21	28.66 0.21	28.66 0.21	24.02	0.000	0.000	0.000
400	6.260	35.88	29.62	25.07	.000	.000	.000
500	10.098	41.55	31.45	25.79	.000	.000	.000
600	12.762	46.31	33.55	26.36	.000	.000	.000
700	14.740	50.41	35.67	26.87	.000	.000	.000
800	16.286	54.03	37.74	27.36	.000	.000	.000
900	17.544	57.28	39.74	27.85	.000	.000	.000
1000	18.601	60.24	41.64	28.38	.000	.000	.000
1100	19.515	62.97	43.46	28.94	.000	.000	.000
1200	20.324	65.51	45.19	29.54	.000	.000	.000
1300	21.058	67.90	46.84	30.19	.000	.000	.000
1400	21.736	70.17	48.43	30.90	.000	.000	.000
1500	22.372	72.32	49.95	31.67	.000	.000	.000
1600	22.978	74.39	51.41	32.50	.000	.000	.000
1700	23.564	76.39	52.83	33.38	.000	.000	.000
1800	24.136	78.32	54.18	34.34	.000	.000	.000

MELTING POINT	2890 K	BOILING POINT	4912 K
ENTHALPY OF MELTING	32.540 kJ	ENTHALPY OF VAPORIZATION	598.070 kJ
$H_{298}^0 - H_0^0$	4.594 kJ	MOLAR VOLUME	0.9387 J/bar 9.387 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

HEAT CAPACITY EQUATION

$$C_P^0 = 34.139 - 4.4926 \times 10^{-3} T + 3.7012 \times 10^{-6} T^2 - 1.5722 \times 10^{-9} T^3 \text{ cal} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-23-76

## NITROGEN (REFERENCE STATE)

FORMULA WEIGHT 28.013

N<sub>2</sub>: Ideal diatomic gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	191.61	191.61	29.12	0.000	0.000	0.000
UNCERTAINTY		0.02	0.02				
400	7.407	200.16	192.75	29.15	.000	.000	.000
500	11.796	206.71	194.91	29.60	.000	.000	.000
600	14.812	212.15	197.34	30.19	.000	.000	.000
700	17.054	216.86	199.81	30.83	.000	.000	.000
800	18.816	221.01	202.19	31.46	.000	.000	.000
900	20.254	224.76	204.51	32.07	.000	.000	.000
1000	21.465	228.16	206.69	32.65	.000	.000	.000
1100	22.506	231.30	208.79	33.19	.000	.000	.000
1200	23.417	234.21	210.79	33.68	.000	.000	.000
1300	24.225	236.92	212.70	34.13	.000	.000	.000
1400	24.946	239.47	214.52	34.53	.000	.000	.000
1500	25.598	241.86	216.26	34.89	.000	.000	.000
1600	26.188	244.13	217.94	35.19	.000	.000	.000
1700	26.725	246.27	219.54	35.45	.000	.000	.000
1800	27.216	248.30	221.08	35.65	.000	.000	.000

MELTING POINT	63.14 K	BOILING POINT	77.35 K
ENTHALPY OF MELTING	0.720 kJ	ENTHALPY OF VAPORIZATION	5.586 kJ
$H_{298}^0 - H_0^0$	8.669 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATION

$$C_P^0 = 23.941 + 1.1068 \times 10^{-2} T - 2.5518 \times 10^{-6} T^2 + 1.9064 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	107	35	COMPILED
	247	247	3-11-76



SODIUM (REFERENCE STATE)

FORMULA WEIGHT 22.990

Na: Body-centered cubic crystals 298.15 to melting point 370.98 K. Liquid 370.98 to fictive boiling point 1175 K. Ideal monatomic gas 1175 to 1800 K. The equilibrium boiling point of the real gas is 1154 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	51.30	51.30	28.23	0.000	0.000	0.000
UNCERTAINTY		0.02	0.02				
370.98	5.808	57.63	51.82	31.97	.000	.000	.000
370.98	12.811	64.63	51.82	31.84	.000	.000	.000
400	14.188	67.15	52.96	31.51	.000	.000	.000
500	17.554	74.07	56.52	30.55	.000	.000	.000
600	19.655	79.57	59.91	29.80	.000	.000	.000
700	21.063	84.13	63.07	29.27	.000	.000	.000
800	22.066	88.01	65.94	28.95	.000	.000	.000
900	22.823	91.41	68.59	28.84	.000	.000	.000
1000	23.428	94.45	71.02	28.94	.000	.000	.000
1100	23.943	97.23	73.29	29.26	.000	.000	.000
1175	24.295	99.15	74.85	29.65	.000	.000	.000
1175	107.367	182.22	74.85	20.79	.000	.000	.000
1200	105.564	182.66	77.10	20.79	.000	.000	.000
1300	99.043	184.32	85.28	20.79	.000	.000	.000
1400	93.453	185.86	92.41	20.79	.000	.000	.000
1500	88.609	187.30	98.69	20.79	.000	.000	.000
1600	84.370	188.64	104.27	20.79	.000	.000	.000
1700	80.630	189.90	109.27	20.90	.000	.000	.000
1800	77.306	191.09	113.78	20.79	.000	.000	.000

MELTING POINT	370.98 K	BOILING POINT	1175 K
ENTHALPY OF MELTING	2.598 kJ	ENTHALPY OF VAPORIZATION	97.610 kJ
$H_{298}^0 - H_0^0$	6.460 kJ	MOLAR VOLUME	2.3812 J/bar 23.812 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 37.482 - 1.9183 \times 10^{-2} T + 1.0644 \times 10^{-5} T^2$$

(EQUATION VALID FROM 370.98 - 1175 K)

REFERENCE 107 35

COMPILED  
7-24-76

NIOBIUM (REFERENCE STATE)

FORMULA WEIGHT 92.906

Nb: Body-centered cubic crystals 298.15 to melting point 2740 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	36.40	36.40	24.70	0.000	0.000	0.000
UNCERTAINTY		0.42	0.42				
400	6.387	43.77	37.38	25.42	.000	.000	.000
500	10.244	49.49	39.25	25.91	.000	.000	.000
600	12.890	54.26	41.37	26.33	.000	.000	.000
700	14.840	58.34	43.50	26.74	.000	.000	.000
800	16.352	61.94	45.59	27.14	.000	.000	.000
900	17.573	65.16	47.59	27.55	.000	.000	.000
1000	18.591	68.08	49.49	27.96	.000	.000	.000
1100	19.461	70.77	51.31	28.37	.000	.000	.000
1200	20.221	73.25	53.03	28.79	.000	.000	.000
1300	20.896	75.58	54.68	29.21	.000	.000	.000
1400	21.505	77.76	56.26	29.63	.000	.000	.000
1500	22.061	79.81	57.75	30.06	.000	.000	.000
1600	22.575	81.77	59.19	30.50	.000	.000	.000
1700	23.054	83.63	60.58	30.93	.000	.000	.000
1800	23.503	85.41	61.91	31.37	.000	.000	.000

MELTING POINT	2740	K	BOILING POINT	5017	K
ENTHALPY OF MELTING	26.368	kJ	ENTHALPY OF VAPORIZATION	682.004	kJ
$H_{298}^0 - H_0^0$	5.251	kJ	MOLAR VOLUME	1.0828 J/bar 10.828 cm <sup>3</sup>	

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 21.778 + 4.6709 \times 10^{-3} T + 51.793 T^{-0.5} - 1.3098 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76

NEODYMIUM (REFERENCE STATE)

FORMULA WEIGHT 144.240

Nd: Alpha crystals (double hexagonal close packed) 298.15 to 1128 K. Beta crystals (body-centered cubic) 1128 to melting point 1289 K. Liquid 1298 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS		
					ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	71.09	71.09	27.45	0.000	0.000	0.000
UNCERTAINTY		4.18	4.18				
400	7.147	79.33	72.18	28.74	.000	.000	.000
500	11.616	85.90	74.28	30.28	.000	.000	.000
600	14.872	91.58	76.71	32.07	.000	.000	.000
700	17.471	96.67	79.20	34.13	.000	.000	.000
800	19.696	101.38	81.68	36.45	.000	.000	.000
900	21.700	105.82	84.12	39.05	.000	.000	.000
1000	23.576	110.08	86.50	41.93	.000	.000	.000
1100	25.386	114.22	88.83	45.09	.000	.000	.000
1128	25.890	115.35	89.45	45.98	.000	.000	.000
1128	28.576	118.03	89.45	44.56	.000	.000	.000
1200	29.537	120.82	91.28	44.56	.000	.000	.000
1289	30.546	118.44	87.89	44.56	.000	.000	.000
1289	36.087	123.98	87.89	48.78	.000	.000	.000
1300	36.195	124.93	88.74	48.78	.000	.000	.000
1400	37.094	133.55	96.46	48.78	.000	.000	.000
1500	37.874	136.91	99.04	48.78	.000	.000	.000
1600	38.556	140.06	101.50	48.78	.000	.000	.000
1700	39.158	143.02	103.86	48.78	.000	.000	.000
1800	39.692	145.81	106.12	48.78	.000	.000	.000

MELTING POINT	1289	K	BOILING POINT	3341	K
ENTHALPY OF MELTING	7.142	kJ	ENTHALPY OF VAPORIZATION	273.040	kJ
$H_{298}^0 - H_0^0$	7.134	kJ	MOLAR VOLUME	2.0570	J/bar
				20.570	cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 29.171 + 1.4652 \times 10^{-5} T^2 - 61.399 T^{-0.5} + 4.7264 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 1128 K)

REFERENCE 107 107

COMPILED  
4-26-76

NEON (REFERENCE STATE)

FORMULA WEIGHT 20.179

Ne: Ideal gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	146.32	146.32	20.79	0.000	0.000	0.000
UNCERTAINTY		0.02	0.02				
400	5.292	152.42	147.13	20.79	.000	.000	.000
500	8.394	157.06	148.67	20.79	.000	.000	.000
600	10.460	160.85	150.39	20.79	.000	.000	.000
700	11.930	164.06	152.13	20.79	.000	.000	.000
800	13.039	166.83	153.80	20.79	.000	.000	.000
900	13.900	169.28	155.38	20.79	.000	.000	.000
1000	14.590	171.47	156.88	20.79	.000	.000	.000
1100	15.154	173.36	158.21	20.79	.000	.000	.000
1200	15.620	175.26	159.64	20.79	.000	.000	.000
1300	16.018	176.86	160.84	20.79	.000	.000	.000
1400	16.359	178.47	162.11	20.79	.000	.000	.000
1500	16.655	179.85	163.20	20.79	.000	.000	.000
1600	16.914	181.24	164.33	20.79	.000	.000	.000
1700	17.139	182.47	165.33	20.79	.000	.000	.000
1800	17.343	183.69	166.35	20.79	.000	.000	.000

MELTING POINT	24.55 K	BOILING POINT	K
ENTHALPY OF MELTING	0.331 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	6.197 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE	107	107	COMPILED 3-11-76
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NICKEL (REFERENCE STATE)

FORMULA WEIGHT 58.700

Ni: Face-centered Curie crystals (magnetic) to Curie point 631 K.

Nonmagnetic 631 to melting point 1726 K. Liquid 1726 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	29.87	29.87	26.06	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	6.962	37.89	30.93	28.45	.000	.000	.000
500	11.484	44.48	33.00	30.88	.000	.000	.000
600	15.022	50.43	35.41	34.89	.000	.000	.000
631	16.066	52.30	36.23	38.91	.000	.000	.000
700	17.614	55.56	37.95	31.01	.000	.000	.000
800	19.274	59.68	40.41	31.00	.000	.000	.000
900	20.622	63.38	42.76	31.89	.000	.000	.000
1000	21.804	66.80	45.00	33.00	.000	.000	.000
1100	22.872	69.99	47.12	34.06	.000	.000	.000
1200	23.842	73.00	49.16	34.94	.000	.000	.000
1300	24.723	75.82	51.10	35.60	.000	.000	.000
1400	25.517	78.48	52.96	36.03	.000	.000	.000
1500	26.227	80.97	54.74	36.26	.000	.000	.000
1600	26.856	83.31	56.45	36.30	.000	.000	.000
1700	27.409	85.51	58.10	36.18	.000	.000	.000
1726	27.535	86.19	58.66	36.19	.000	.000	.000
1726	37.658	96.32	58.66	43.10	.000	.000	.000
1800	37.879	98.12	60.25	43.10	.000	.000	.000

MELTING POINT	1726 K	BOILING POINT	3187 K
ENTHALPY OF MELTING	17.472 kJ	ENTHALPY OF VAPORIZATION	370.380 kJ
$H_{298}^0 - H_0^0$	4.786 kJ	MOLAR VOLUME	0.6588 J/bar 6.588 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.5135 \times 10^2 - 0.20499 T + 1.7411 \times 10^{-4} T^2 - 1.3753 \times 10^{-8} T^{0.5}$$

(EQUATION VALID FROM 298 - 631 K)

$$C_P^0 = 3.0548 \times 10^2 - 7.0339 \times 10^{-2} T + 7.5973 \times 10^{-6} T^2 - 7.4450 \times 10^{-9} T^{0.5}$$

$$2.5697 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 631 - 1726 K)

REFERENCE 107 107

COMPILED  
5-11-76

OXYGEN (REFERENCE STATE)

FORMULA WEIGHT 31.999

O<sub>2</sub>: Ideal diatomic gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	205.15	205.15	29.37	0.000	0.000	0.000
UNCERTAINTY		0.04	0.04				
400	7.560	213.87	206.31	30.13	.000	.000	.000
500	12.176	220.70	208.52	31.16	.000	.000	.000
600	15.420	226.47	211.05	32.12	.000	.000	.000
700	17.867	231.48	213.61	32.95	.000	.000	.000
800	19.799	235.93	216.13	33.67	.000	.000	.000
900	21.376	239.94	218.56	34.29	.000	.000	.000
1000	22.694	243.58	220.89	34.82	.000	.000	.000
1100	23.818	246.92	223.10	35.29	.000	.000	.000
1200	24.792	250.01	225.22	35.69	.000	.000	.000
1300	25.644	252.88	227.24	36.05	.000	.000	.000
1400	26.399	255.56	229.16	36.36	.000	.000	.000
1500	27.072	258.08	231.01	36.64	.000	.000	.000
1600	27.678	260.45	232.77	36.89	.000	.000	.000
1700	28.226	262.69	234.46	37.11	.000	.000	.000
1800	28.726	264.82	236.09	37.31	.000	.000	.000

MELTING POINT	54.35 K	BOILING POINT	90.18 K
ENTHALPY OF MELTING	0.444 kJ	ENTHALPY OF VAPORIZATION	6.816 kJ
$H_{298}^0 - H_0^0$	8.682 kJ	MOLAR VOLUME	2478.92 00 J/bar 24789.200 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 48.318 - 6.9132 \times 10^{-4} T - 4.2066 \times 10^{-2} T^{-0.5} + 4.9923 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107

35

COMPILED  
3-11-76

OSMIUM (REFERENCE STATE)

FORMULA WEIGHT 190.200

Os: Hexagonal close packed crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	32.64	32.64	24.71	0.000	0.000	0.000
UNCERTAINTY		0.06	0.06				
400	6.340	39.95	33.61	25.09	.000	.000	.000
500	10.130	45.60	35.47	25.48	.000	.000	.000
600	12.718	50.27	37.55	25.86	.000	.000	.000
700	14.623	54.29	39.67	26.24	.000	.000	.000
800	16.099	57.82	41.72	26.62	.000	.000	.000
900	17.288	60.97	43.68	27.00	.000	.000	.000
1000	18.278	63.84	45.56	27.38	.000	.000	.000
1100	19.123	66.47	47.35	27.76	.000	.000	.000
1200	19.858	68.90	49.04	28.14	.000	.000	.000
1300	20.511	71.16	50.65	28.52	.000	.000	.000
1400	21.096	73.29	52.19	28.90	.000	.000	.000
1500	21.629	75.30	53.67	29.28	.000	.000	.000
1600	22.120	77.20	55.08	29.66	.000	.000	.000
1700	22.575	79.01	56.44	30.05	.000	.000	.000
1800	23.001	80.74	57.74	30.43	.000	.000	.000

MELTING POINT	3300 K	BOILING POINT	5285 K
ENTHALPY OF MELTING	31.757 kJ	ENTHALPY OF VAPORIZATION	746.080 kJ
$H_{298}^0 - H_0^0$		MOLAR VOLUME	0.8423 J/bar 8.423 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 23.571 + 3.8083 \times 10^{-3} T$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107 COMPILED 4-17-76

## PHOSPHORUS (REFERENCE STATE)

FORMULA WEIGHT 30.974

P: Crystals (red triclinic, V) 298.15 K to sublimation point 704 K. Ideal diatomic gas 704 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	22.85	22.85	21.21	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	5.670	29.38	23.71	23.16	.000	.000	.000
500	9.314	34.70	25.39	24.51	.000	.000	.000
600	11.952	39.28	27.33	25.79	.000	.000	.000
700	14.029	43.36	29.33	27.19	.000	.000	.000
704	14.104	43.52	29.42	27.25	.000	.000	.000
704	136.781	123.83	-12.95	18.01	.000	.000	.000
800	122.539	126.14	3.60	18.18	.000	.000	.000
900	110.950	128.29	17.34	18.31	.000	.000	.000
1000	101.692	130.22	28.53	18.41	.000	.000	.000
1100	94.125	131.98	37.86	18.50	.000	.000	.000
1200	87.826	133.59	45.77	18.59	.000	.000	.000
1300	82.498	135.08	52.58	18.68	.000	.000	.000
1400	77.936	136.46	58.53	18.78	.000	.000	.000
1500	73.984	137.75	63.77	18.90	.000	.000	.000
1600	70.529	138.96	68.43	19.03	.000	.000	.000
1700	67.483	140.09	72.61	19.18	.000	.000	.000
1800	64.775	141.17	76.39	19.36	.000	.000	.000

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	3.607 kJ	MOLAR VOLUME	1.7200 J/bar 17.200 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATIONS

$$C_p^0 = 35.859 - 1.6031 \times 10^{-2} T + 1.8309 \times 10^{-5} T^2 - 1.5866 \times 10^{-8} T^3 - 2.0482 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 704 K)

$$C_p^0 = 30.350 - 6.3500 \times 10^{-3} T + 1.8664 \times 10^{-6} T^2 - 2.3929 \times 10^{-9} T^3 + 1.1167 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 704 - 1800 K)

REFERENCE 107 107

COMPILED  
8-18-76



LEAD (REFERENCE STATE)

FORMULA WEIGHT 207.200

Pb: Face-centered cubic crystals 298.15 to melting point 600.6 K. Liquid  
600.6 to boiling point 2021 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	65.06	65.06	26.61	0.000	0.000	0.000
UNCERTAINTY		0.42	0.42				
400	6.872	72.99	66.12	27.40	.000	.000	.000
500	11.070	79.20	68.13	28.33	.000	.000	.000
600	14.033	84.46	70.43	29.39	.000	.000	.000
600.6	14.088	85.14	71.06	29.40	.000	.000	.000
600.6	22.078	93.13	71.06	30.58	.000	.000	.000
700	23.233	97.14	73.91	30.37	.000	.000	.000
800	24.165	101.17	77.07	30.03	.000	.000	.000
900	24.743	104.69	79.95	29.68	.000	.000	.000
1000	25.220	107.80	82.58	29.35	.000	.000	.000
1100	25.584	110.58	85.00	29.08	.000	.000	.000
1200	25.866	113.10	87.23	28.87	.000	.000	.000
1300	26.090	115.41	89.32	28.71	.000	.000	.000
1400	26.273	117.53	91.26	28.60	.000	.000	.000
1500	26.426	119.50	93.07	28.54	.000	.000	.000
1600	26.557	121.34	94.78	28.52	.000	.000	.000
1700	26.674	123.07	96.40	28.55	.000	.000	.000
1800	26.779	124.71	97.93	28.60	.000	.000	.000

MELTING POINT	600.6 K	BOILING POINT	2021 K
ENTHALPY OF MELTING	4.799 kJ	ENTHALPY OF VAPORIZATION	177.699 kJ
$H_{298}^0 - H_0^0$	6.874 kJ	MOLAR VOLUME	1.8267 J/bar 18.267 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 13.743 + 1.5675 \times 10^{-2} T + 1.5920 \times 10^{-5} T^{-0.5} - 9.1526 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 600.6 K)

$$C_P^0 = 5.3727 \times 10^{-3} T + 8.3501 \times 10^{-6} T^{-0.5} - 2.4248 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 600.60 - 1800 K)

REFERENCE 107 107

COMPILED  
4-10-76

PALLADIUM (REFERENCE STATE)

FORMULA WEIGHT 106.400

Pd: Face-centered cubic crystals 298.15 to melting point 1825 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	37.82	37.82	25.93	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.710	45.56	38.85	26.73	.000	.000	.000
500	10.774	51.59	40.82	27.32	.000	.000	.000
600	13.575	56.61	43.04	27.83	.000	.000	.000
700	15.647	60.94	45.29	28.32	.000	.000	.000
800	17.260	64.75	47.49	28.79	.000	.000	.000
900	18.569	68.17	49.60	29.28	.000	.000	.000
1000	19.665	71.28	51.61	29.79	.000	.000	.000
1100	20.610	74.15	53.54	30.33	.000	.000	.000
1200	21.443	76.81	55.37	30.90	.000	.000	.000
1300	22.193	79.31	57.12	31.51	.000	.000	.000
1400	22.881	81.67	58.79	32.15	.000	.000	.000
1500	23.522	83.91	60.39	32.84	.000	.000	.000
1600	24.127	86.05	61.92	33.57	.000	.000	.000
1700	24.705	88.11	63.41	34.34	.000	.000	.000
1800	25.263	90.09	64.83	35.16	.000	.000	.000

MELTING POINT	1825 K	BOILING POINT	3237 K
ENTHALPY OF MELTING	17.560 kJ	ENTHALPY OF VAPORIZATION	357.510 kJ
$H_{298}^0 - H_0^0$	5.469 kJ	MOLAR VOLUME	0.8862 J/bar 8.862 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 31.615 - 1.3625 \times 10^{-3} T + 2.5427 \times 10^{-6} T^2 - 95.020 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76

PRASEODYMIUM (REFERENCE STATE)

FORMULA WEIGHT 140.908

Pr: Alpha crystals (double hexagonal close packed) 298.15 to 1068 K. Beta crystals (body-centered cubic) 1068 to 1204 K. Liquid 1204 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>p</sub> <sup>0</sup> J/mol·K			
298.15	0.000	73.93	73.93	27.44	0.000	0.000	0.000
UNCERTAINTY		4.18	4.18				
400	7.092	82.11	75.02	28.37	.000	.000	.000
500	11.480	88.58	77.10	29.77	.000	.000	.000
600	14.670	94.16	79.49	31.50	.000	.000	.000
700	17.213	99.16	81.95	33.47	.000	.000	.000
800	19.377	103.77	84.39	35.62	.000	.000	.000
900	21.307	108.09	86.78	37.88	.000	.000	.000
1000	23.082	112.21	89.13	40.24	.000	.000	.000
1068	24.099	114.85	90.75	41.90	.000	.000	.000
1068	27.183	117.93	90.75	38.45	.000	.000	.000
1100	27.512	119.00	91.49	38.45	.000	.000	.000
1200	28.427	122.35	93.92	38.45	.000	.000	.000
1204	28.463	122.73	94.26	38.45	.000	.000	.000
1204	34.183	128.45	94.26	42.97	.000	.000	.000
1300	34.832	131.50	96.67	42.97	.000	.000	.000
1400	35.413	134.68	99.27	42.97	.000	.000	.000
1500	35.917	137.64	101.72	42.97	.000	.000	.000
1600	36.357	140.42	104.06	42.97	.000	.000	.000
1700	36.746	143.02	106.27	42.97	.000	.000	.000
1800	37.092	145.48	108.39	42.97	.000	.000	.000

MELTING POINT	1204 K	BOILING POINT	3785 K
ENTHALPY OF MELTING	6.887 kJ	ENTHALPY OF VAPORIZATION	296.780 kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	7.418 kJ	MOLAR VOLUME	2.0800 J/bar 20.800 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 2.9291 \times 10^{-2} T + 3.5092 \times 10^{-5} T^{-0.5} - 1.4325 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1068 K)

REFERENCE 107 107

COMPILED  
4-26-76

PLATINUM (REFERENCE STATE)

FORMULA WEIGHT 195.090

Pt: Face-centered cubic crystals 298.15 to melting point 2042 K.

TEMP. K	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	41.63	41.63	25.81	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.665	49.32	42.65	26.49	.000	.000	.000
500	10.684	55.29	44.61	27.02	.000	.000	.000
600	13.450	60.26	46.81	27.53	.000	.000	.000
700	15.497	64.54	49.04	28.04	.000	.000	.000
800	17.097	68.32	51.22	28.56	.000	.000	.000
900	18.400	71.71	53.31	29.08	.000	.000	.000
1000	19.494	74.80	55.31	29.61	.000	.000	.000
1100	20.439	77.65	57.21	30.15	.000	.000	.000
1200	21.270	80.30	59.03	30.69	.000	.000	.000
1300	22.015	82.77	60.76	31.22	.000	.000	.000
1400	22.691	85.11	62.42	31.76	.000	.000	.000
1500	23.313	87.32	64.01	32.29	.000	.000	.000
1600	23.891	89.42	65.53	32.82	.000	.000	.000
1700	24.431	91.42	66.99	33.34	.000	.000	.000
1800	24.941	93.34	68.40	33.86	.000	.000	.000

MELTING POINT	2042 K	BOILING POINT	4100 K
ENTHALPY OF MELTING	19.648 kJ	ENTHALPY OF VAPORIZATION	509.820 kJ
$H_{298}^0 - H_0^0$	5.724 kJ	MOLAR VOLUME	6.9091 J/bar 9.091 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 20.046 + 7.4148 \times 10^{-3} T - 4.7980 \times 10^{-7} T^2 + 87.382 T^{-0.5}$$

$$-1.2980 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76

PLUTONIUM (REFERENCE STATE) FORMULA WEIGHT 244.002

Pu: Alpha crystals (monoclinic, simple) 298.15 to 395 K. Beta crystals (body-centered monoclinic) 395 to 480 K. Gamma crystals (face-centered orthorhombic) 480 to 588 K. Delta crystals (face-centered cubic) 588 to 730 K. Delta prime crystals (body-centered tetragonal) 730 to 753 K. Epsilon crystals (bcc) 753 to 913 K. Liquid 913 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	51.46	51.46	31.97	0.000	0.000	0.000
UNCERTAINTY							
		8.37	8.37				
395	8.177	60.84	52.68	34.31	.000	.000	.000
395	16.651	69.33	52.68	33.47	.000	.000	.000
400	16.862	69.74	52.88	28.46	.000	.000	.000
480	19.848	76.11	56.28	35.98	.000	.000	.000
480	21.068	77.32	56.28	34.73	.000	.000	.000
500	21.632	78.74	57.11	35.69	.000	.000	.000
588	24.037	84.85	60.84	39.75	.000	.000	.000
588	24.962	85.77	60.84	37.66	.000	.000	.000
600	25.215	86.52	61.31	37.66	.000	.000	.000
700	26.993	92.34	65.35	37.66	.000	.000	.000
730	27.431	93.93	66.53	37.66	.000	.000	.000
730	27.546	94.06	66.53	37.66	.000	.000	.000
753	27.854	95.19	67.32	37.66	.000	.000	.000
753	30.299	97.61	67.32	35.15	.000	.000	.000
800	30.585	99.74	69.16	35.15	.000	.000	.000
900	31.092	103.89	72.79	35.15	.000	.000	.000
913	31.162	104.86	73.70	35.15	.000	.000	.000
913	34.278	107.98	73.70	41.84	.000	.000	.000
1000	34.936	111.29	76.35	41.84	.000	.000	.000
1100	35.564	115.10	79.54	41.84	.000	.000	.000
1200	36.087	118.91	82.82	41.84	.000	.000	.000
1300	36.529	122.15	85.62	41.84	.000	.000	.000
1400	36.909	125.39	88.48	41.84	.000	.000	.000
1500	37.057	128.17	91.12	41.84	.000	.000	.000
1600	37.525	130.96	93.43	41.84	.000	.000	.000
1700	37.779	133.42	95.65	41.84	.000	.000	.000
1800	38.004	135.89	97.89	41.84	.000	.000	.000

MELTING POINT 913 K BOILING POINT 3503 K

ENTHALPY OF MELTING 2.845 kJ ENTHALPY OF VAPORIZATION 343.670 kJ

$H_{298}^0 - H_0^0$  6.485 kJ MOLAR VOLUME 1.2040 J/bar  
   12.040 cm<sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE 107 107 COMPILED  
5-15-73

## RUBIDIUM (REFERENCE STATE)

FORMULA WEIGHT 85.468

Rb: Body-centered cubic 298.15 to melting point 312.64 K. Liquid 312.64 to boiling point 959 K. Ideal monatomic gas 959 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	76.78	76.78	31.06	0.000	0.000	0.000
UNCERTAINTY		0.30	0.30				
312.64	1.472	78.28	76.80	32.40	.000	.000	.000
312.64	8.485	85.30	76.80	34.40	.000	.000	.000
400	13.977	93.59	79.61	32.88	.000	.000	.000
500	17.610	100.77	83.16	31.45	.000	.000	.000
600	19.818	106.40	86.58	30.33	.000	.000	.000
700	21.257	111.01	89.75	29.51	.000	.000	.000
800	22.252	114.92	92.67	28.99	.000	.000	.000
900	22.988	118.31	95.32	28.79	.000	.000	.000
959	23.341	120.13	96.79	28.67	.000	.000	.000
959	97.577	194.37	96.79	20.79	.000	.000	.000
1000	94.428	195.24	100.81	20.79	.000	.000	.000
1100	87.735	197.22	109.48	20.79	.000	.000	.000
1200	82.156	199.03	116.87	20.79	.000	.000	.000
1300	77.435	200.69	123.26	20.79	.000	.000	.000
1400	73.389	202.23	128.84	20.79	.000	.000	.000
1500	69.883	203.66	133.78	20.79	.000	.000	.000
1600	66.814	205.01	138.20	20.79	.000	.000	.000
1700	64.107	206.27	142.16	20.79	.000	.000	.000
1800	61.701	207.45	145.75	20.79	.000	.000	.000

MELTING POINT	312.64 K	BOILING POINT	959 K
ENTHALPY OF MELTING	2.192 kJ	ENTHALPY OF VAPORIZATION	71.192 kJ
$H_{298}^0 - H_0^0$	7.489 kJ	MOLAR VOLUME	5.5850 J/bar 55.850 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATION

$$C_P^0 = 41.678 - 2.8113 \times 10^{-2} T + 1.5320 \times 10^{-5} T^2$$

(EQUATION VALID FROM 312.64 - 959 K)

REFERENCE 107 35

COMPILED  
4-10-76

RHENIUM (REFERENCE STATE)

FORMULA WEIGHT 186.207

Re: Hexagonal close packed crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	36.53	36.53	25.16	0.000	0.000	0.000
UNCERTAINTY		0.38	0.38				
400	6.510	44.04	37.53	25.92	.000	.000	.000
500	10.450	49.88	39.43	26.49	.000	.000	.000
600	13.168	54.76	41.59	27.01	.000	.000	.000
700	15.183	58.96	43.78	27.53	.000	.000	.000
800	16.757	62.67	45.91	28.05	.000	.000	.000
900	18.041	66.01	47.97	28.57	.000	.000	.000
1000	19.121	69.04	49.92	29.10	.000	.000	.000
1100	20.052	71.84	51.79	29.63	.000	.000	.000
1200	20.873	74.44	53.57	30.17	.000	.000	.000
1300	21.609	76.88	55.27	30.72	.000	.000	.000
1400	22.280	79.18	56.90	31.27	.000	.000	.000
1500	22.898	81.35	58.45	31.83	.000	.000	.000
1600	23.473	83.43	59.96	32.38	.000	.000	.000
1700	24.014	85.41	61.40	32.94	.000	.000	.000
1800	24.526	87.31	62.78	33.51	.000	.000	.000

MELTING POINT	3453 K	BOILING POINT	5869 K
ENTHALPY OF MELTING	33.229 kJ	ENTHALPY OF VAPORIZATION	714.840 kJ
$H_{298}^0 - H_0^0$	5.355 kJ	MOLAR VOLUME	0.8860 J/bar 8.860 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 21.470 + 5.9728 \times 10^{-3} T + 56.132 T^{-0.5} - 1.1928 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76

RHODIUM (REFERENCE STATE)

FORMULA WEIGHT 102.906

Rh: Face-centered cubic crystals 298.15 to melting point 2233 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	31.54	31.54	24.95	0.000	0.000	0.000
UNCERTAINTY							
		0.21	0.21				
400	6.515	39.05	32.53	26.15	.000	.000	.000
500	10.540	44.99	34.45	27.14	.000	.000	.000
600	13.388	50.03	36.64	28.11	.000	.000	.000
700	15.560	54.43	38.87	29.08	.000	.000	.000
800	17.311	58.38	41.07	30.05	.000	.000	.000
900	18.780	61.97	43.19	31.01	.000	.000	.000
1000	20.049	65.29	45.24	31.93	.000	.000	.000
1100	21.171	68.37	47.20	32.83	.000	.000	.000
1200	22.177	71.27	49.09	33.68	.000	.000	.000
1300	23.095	74.00	50.91	34.49	.000	.000	.000
1400	23.936	76.58	52.64	35.25	.000	.000	.000
1500	24.714	79.04	54.33	35.96	.000	.000	.000
1600	25.437	81.38	55.94	36.61	.000	.000	.000
1700	26.112	83.61	57.50	37.20	.000	.000	.000
1800	26.743	85.76	59.02	37.73	.000	.000	.000

MELTING POINT	2233 K	BOILING POINT	3970 K
ENTHALPY OF MELTING	21.489 kJ	ENTHALPY OF VAPORIZATION	493.260 kJ
$H_{298}^0 - H_0^0$	4.920 kJ	MOLAR VOLUME	0.8282 J/bar 8.282 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 8.9772 + 1.9571 \times 10^{-2} T - 3.6535 \times 10^{-6} T^2 + 2.3075 \times 10^{-9} T^3 - 2.5759 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76



RADON (REFERENCE STATE)

FORMULA WEIGHT 222.000

Rn: Ideal gas 298.15 to 1800 K.

FORMATION FROM THE ELEMENTS  
GIBBS

TEMP.	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	176.23	176.23	20.79	0.000	0.000	0.000
UNCERTAINTY		0.00	0.00				
400	5.292	182.34	177.05	20.79	.000	.000	.000
500	8.392	186.98	178.59	20.79	.000	.000	.000
600	10.457	190.77	180.31	20.79	.000	.000	.000
700	11.933	193.97	182.04	20.79	.000	.000	.000
800	13.040	196.75	183.71	20.79	.000	.000	.000
900	13.900	199.19	185.29	20.79	.000	.000	.000
1000	14.589	201.38	186.79	20.79	.000	.000	.000
1100	15.152	203.37	188.22	20.79	.000	.000	.000
1200	15.622	205.17	189.55	20.79	.000	.000	.000
1300	16.019	206.84	190.82	20.79	.000	.000	.000
1400	16.359	208.38	192.02	20.79	.000	.000	.000
1500	16.655	209.81	193.16	20.79	.000	.000	.000
1600	16.912	211.15	194.24	20.79	.000	.000	.000
1700	17.141	212.41	195.27	20.79	.000	.000	.000
1800	17.343	213.60	196.26	20.79	.000	.000	.000

MELTING POINT 202 K BOILING POINT 211 K

ENTHALPY OF MELTING 2.887 kJ ENTHALPY OF VAPORIZATION 16.405 kJ

$H_{298}^0 - H_0^0$  kJ MOLAR VOLUME 2478.9200 J/bar  
24789.200  $\text{cm}^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE 107 107

COMPILED  
4-17-76

RUTHENIUM (REFERENCE STATE)

FORMULA WEIGHT 101.070

Ru: Hexagonal close packed crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	28.53	28.53	24.05	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.155	35.63	29.47	24.37	.000	.000	.000
500	9.848	41.12	31.27	24.88	.000	.000	.000
600	12.400	45.71	33.31	25.45	.000	.000	.000
700	14.307	49.68	35.37	26.05	.000	.000	.000
800	15.812	53.20	37.39	26.67	.000	.000	.000
900	17.056	56.37	39.31	27.32	.000	.000	.000
1000	18.115	59.29	41.18	28.00	.000	.000	.000
1100	19.046	61.99	42.94	28.72	.000	.000	.000
1200	19.883	64.52	44.64	29.47	.000	.000	.000
1300	20.651	66.91	46.26	30.26	.000	.000	.000
1400	21.367	69.18	47.81	31.10	.000	.000	.000
1500	22.045	71.36	49.32	31.98	.000	.000	.000
1600	22.694	73.45	50.76	32.90	.000	.000	.000
1700	23.322	75.47	52.15	33.87	.000	.000	.000
1800	23.936	77.44	53.50	34.88	.000	.000	.000

MELTING POINT	2523 K	BOILING POINT	4423 K
ENTHALPY OF MELTING	24.280 kJ	ENTHALPY OF VAPORIZATION	595.540 kJ
$H_{298}^0 - H_0^0$	4.602 kJ	MOLAR VOLUME	0.8171 J/bar 8.171 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 29.062 + 2.6805 \times 10^{-6} T^2 - 1.2368 \times 10^{-9} T^{0.5} + 1.6966 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76

SULFUR (REFERENCE STATE) FORMULA WEIGHT 32.060

S: Orthorhombic crystals 298.15 to 368.54 K. Monoclinic crystals 368.54 to melting point 388.36 K. Liquid 388.36 to boiling point 716.9 K. Ideal diatomic gas 716.9 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	31.80	31.80	22.72	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
368.54	4.484	36.76	32.28	24.18	.000	.000	.000
368.54	5.574	37.85	32.28	24.74	.000	.000	.000
388.36	6.561	39.75	33.19	25.33	.000	.000	.000
388.36	10.978	44.17	33.19	31.71	.000	.000	.000
400	11.620	45.09	33.47	32.27	.000	.000	.000
500	17.146	53.94	36.80	38.05	.000	.000	.000
600	20.285	60.43	40.14	34.33	.000	.000	.000
700	22.146	65.59	43.45	32.61	.000	.000	.000
716.9	22.382	66.34	43.96	32.19	.000	.000	.000
716.9	100.238	129.26	29.02	18.14	.000	.000	.000
800	91.676	131.27	39.59	18.28	.000	.000	.000
900	83.527	133.44	49.91	18.39	.000	.000	.000
1000	77.019	135.38	58.36	18.48	.000	.000	.000
1100	71.703	137.14	65.44	18.56	.000	.000	.000
1200	67.275	138.76	71.49	18.62	.000	.000	.000
1300	63.532	140.26	76.73	18.67	.000	.000	.000
1400	60.330	141.64	81.31	18.70	.000	.000	.000
1500	57.558	142.93	85.37	18.74	.000	.000	.000
1600	55.132	144.14	89.01	18.78	.000	.000	.000
1700	52.994	145.28	92.29	18.80	.000	.000	.000
1800	51.096	146.36	95.26	18.83	.000	.000	.000

MELTING POINT	388.36 K	BOILING POINT	716.9 K
ENTHALPY OF MELTING	1.715 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	4.410 kJ	MOLAR VOLUME	1.5511 J/bar 15.511 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 23.535 - 1.7230 \times 10^{-3} T + 3.4702 \times 10^{-7} T^2 - 1.1562 \times 10^2 T^{-0.5} - 1.1320 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 716.9 - 1800 K)

REFERENCE 247 247 COMPILED  
5-24-76

## DIATOMIC SULFUR

FORMULA WEIGHT 64.120

S<sub>2</sub>: Ideal diatomic gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS							
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	228.17	228.17	32.46	128.490	79.453	-13.920	
UNCERTAINTY		0.05	0.05		0.500	0.669	0.117	
400	8.492	237.96	229.47	34.10	122.591	63.477	-8.289	
500	13.720	245.68	231.96	35.09	118.204	49.306	-5.151	
600	17.340	252.14	234.80	35.75	114.552	35.780	-3.115	
700	20.004	257.69	237.69	36.21	111.489	22.938	-1.712	
800	22.051	262.55	240.50	36.55	.000	.000	.000	
900	23.677	266.87	243.19	36.79	.000	.000	.000	
1000	24.998	270.75	245.75	36.98	.000	.000	.000	
1100	26.095	274.29	248.20	37.13	.000	.000	.000	
1200	27.019	277.52	250.50	37.24	.000	.000	.000	
1300	27.809	280.51	252.70	37.34	.000	.000	.000	
1400	28.492	283.28	254.79	37.41	.000	.000	.000	
1500	29.089	285.86	256.77	37.48	.000	.000	.000	
1600	29.616	288.28	258.66	37.54	.000	.000	.000	
1700	30.084	290.56	260.48	37.60	.000	.000	.000	
1800	30.503	292.71	262.21	37.66	.000	.000	.000	

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	9.131 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 47.069 - 3.4459 \times 10^{-3} T + 6.9404 \times 10^{-7} T^2 - 2.3124 \times 10^{-2} T^{-0.5} - 2.2639 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 247 247

COMPILED  
8-12-76

OCTA-ATOMIC SULFUR

FORMULA WEIGHT 256.480

S<sub>8</sub>: Ideal octatomic gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	430.32	430.32	156.04	101.253	48.836	-8.556
UNCERTAINTY		1.67	1.67		0.628	0.920	0.161
400	41.290	477.90	436.61	166.86	80.585	33.707	-4.402
500	66.984	515.75	448.77	172.15	66.161	24.054	-2.513
600	84.788	547.44	462.65	175.23	54.758	16.344	-1.423
700	97.859	574.61	476.75	177.18	45.738	10.837	-0.809
800	107.861	598.36	490.50	178.50	-399.186	-38.015	2.482
900	115.763	619.44	503.68	179.42	-395.952	7.306	-0.424
1000	122.164	638.38	516.22	180.09	-392.735	51.957	-2.714
1100	127.454	655.56	528.11	180.50	-389.532	96.228	-4.570
1200	131.897	671.29	539.39	180.95	-386.311	140.285	-6.106
1300	135.682	685.79	550.11	181.23	-383.097	184.059	-7.396
1400	138.943	699.23	560.29	181.46	-379.923	227.557	-8.490
1500	141.783	711.75	569.97	181.64	-376.768	270.791	-9.430
1600	144.279	723.48	579.20	181.78	-373.589	313.899	-10.248
1700	146.489	734.51	588.02	181.91	-370.436	356.746	-10.962
1800	148.459	744.91	596.45	182.02	-367.304	399.428	-11.591

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	31.330 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 2.0004 \times 10^2 - 6.4724 \times 10^{-3} T + 1.1897 \times 10^{-6} T^2 - 4.1246 \times 10^2 T^{-0.5} - 1.6260 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 247 247 COMPILED 8-12-76

## ANTIMONY (REFERENCE STATE)

FORMULA WEIGHT 121.750

Sb: Rhombohedral crystals 298.15 to melting point 904 K. Liquid 904 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	45.52	45.52	25.26	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.517	53.04	46.52	25.91	.000	.000	.000
500	10.454	58.88	48.43	26.48	.000	.000	.000
600	13.178	63.77	50.59	27.16	.000	.000	.000
700	15.239	68.02	52.78	28.09	.000	.000	.000
800	16.919	71.85	54.93	29.32	.000	.000	.000
900	18.381	75.39	57.01	30.92	.000	.000	.000
904	18.411	75.54	57.11	30.99	.000	.000	.000
904	40.424	97.53	57.11	31.38	.000	.000	.000
1000	39.556	100.68	61.12	31.38	.000	.000	.000
1100	38.813	103.67	64.86	31.38	.000	.000	.000
1200	38.193	106.40	68.21	31.38	.000	.000	.000
1300	37.669	108.91	71.24	31.38	.000	.000	.000
1400	37.220	111.24	74.02	31.38	.000	.000	.000
1500	36.831	113.40	76.57	31.38	.000	.000	.000
1600	36.490	115.43	78.94	31.38	.000	.000	.000
1700	36.189	117.33	81.14	31.38	.000	.000	.000
1800	35.922	119.12	83.20	31.38	.000	.000	.000

MELTING POINT	904 K	BOILING POINT	1860 K
ENTHALPY OF MELTING	19.874 kJ	ENTHALPY OF VAPORIZATION	86.525 kJ
$H_{298}^0 - H_0^0$	5.870 kJ	MOLAR VOLUME	1.8178 J/bar 18.178 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 52.624 - 3.2992 \times 10^{-2} T + 2.4691 \times 10^{-5} T^2 - 3.6512 \times 10^{-8} T^{-0.5} \\ 1.2617 \times 10^5 T^{-2} \\ \text{(EQUATION VALID FROM 298 - 904 K)}$$

REFERENCE 107 107

COMPILED  
4-13-76

SCANDIUM (REFERENCE STATE) FORMULA WEIGHT 44.956

Sc: Alpha crystals (hexagonal close packed) 298.15 to 1608 K. Beta crystals  
(body-centered cubic) 1608 to 1812 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	34.64	34.64	25.45	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.592	42.24	35.65	26.26	.000	.000	.000
500	10.588	48.17	37.58	26.86	.000	.000	.000
600	13.353	53.12	39.77	27.51	.000	.000	.000
700	15.429	57.42	41.99	28.27	.000	.000	.000
800	17.086	61.25	44.16	29.13	.000	.000	.000
900	18.478	64.74	46.26	30.11	.000	.000	.000
1000	19.695	67.96	48.27	31.20	.000	.000	.000
1100	20.795	70.99	50.20	32.41	.000	.000	.000
1200	21.816	73.87	52.05	33.71	.000	.000	.000
1300	22.785	76.62	53.84	35.12	.000	.000	.000
1400	23.719	79.28	55.56	36.63	.000	.000	.000
1500	24.633	81.86	57.23	38.24	.000	.000	.000
1600	25.536	84.38	58.84	39.95	.000	.000	.000
1608	25.604	84.58	58.98	40.09	.000	.000	.000
1608	28.105	87.08	58.98	44.22	.000	.000	.000
1700	28.974	89.54	60.57	44.22	.000	.000	.000
1800	29.818	92.06	62.24	44.22	.000	.000	.000

MELTING POINT	1812 K	BOILING POINT	3104 K
ENTHALPY OF MELTING	14.096 kJ	ENTHALPY OF VAPORIZATION	314.190 kJ
$H_{298}^0 - H_0^0$	5.217 kJ	MOLAR VOLUME	1.5038 J/bar 15.038 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 17.475 + 4.7392 \times 10^{-3} T + 4.3418 \times 10^{-6} T^2 + 1.5482 \times 10^{-9} T^3 - 2.4760 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1608 K)

REFERENCE 107 107 COMPILED  
4-12-76

SELENIUM (REFERENCE STATE) FORMULA WEIGHT 78.960

Se: Crystals 298.15 to melting point 494 K. Liquid 494 to boiling point  
957 K. Ideal diatomic gas 957 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	42.27	42.27	25.06	0.000	0.000	0.000
UNCERTAINTY		0.05	0.05				
400	6.556	49.826	43.27	26.44	.000	.000	.000
494	10.446	55.51	45.06	27.30	.000	.000	.000
494	22.906	67.97	45.06	35.95	.000	.000	.000
500	23.056	68.38	45.32	35.85	.000	.000	.000
600	25.070	74.79	49.72	34.37	.000	.000	.000
700	26.339	80.03	53.69	33.54	.000	.000	.000
800	27.214	84.48	57.27	33.29	.000	.000	.000
900	27.917	88.43	60.51	33.93	.000	.000	.000
957	28.305	90.50	62.19	34.78	.000	.000	.000
957	84.275	146.44	62.19	19.27	.000	.000	.000
1000	81.481	147.29	65.81	19.31	.000	.000	.000
1100	75.834	149.13	73.30	19.41	.000	.000	.000
1200	71.136	150.82	79.68	19.52	.000	.000	.000
1300	67.169	162.39	85.22	19.62	.000	.000	.000
1400	63.776	153.84	90.06	19.73	.000	.000	.000
1500	60.843	155.21	94.37	19.83	.000	.000	.000
1600	58.283	156.49	98.21	19.94	.000	.000	.000
1700	56.028	157.70	101.67	20.04	.000	.000	.000
1800	54.031	158.85	104.82	20.15	.000	.000	.000

MELTING POINT	494 K	BOILING POINT	957 K
ENTHALPY OF MELTING	6.159 kJ	ENTHALPY OF VAPORIZATION	53.563 kJ
$H_{298}^0 - H_0^0$	5.519 kJ	MOLAR VOLUME	1.6420 J/bar 16.420 $\text{cm}^3$
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATIONS

$$C_p^0 = -4.5189 \times 10^2 + 0.67669 T - 4.3675 \times 10^{-4} T^2 + 5.8695 \times 10^3 T^{-0.5} - 2.3024 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 494 K)

$$C_p^0 = 1.1612 \times 10^{-2} T - 2.9520 \times 10^{-6} T^2 + 3.4519 \times 10^2 T^{-0.5} - 2.6879 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 957 - 1800 K)

REFERENCE 75 30

COMPILED  
4-30-76



SILICON (REFERENCE STATE)

FORMULA WEIGHT 28.086

Si: Crystals 298.15 to melting point 1685 K. Liquid 1685 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	18.81	18.81	19.94	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	5.385	25.01	19.62	22.15	.000	.000	.000
500	8.880	30.10	21.22	23.47	.000	.000	.000
600	11.393	34.7	23.08	24.40	.000	.000	.000
700	13.303	38.29	24.99	25.10	.000	.000	.000
800	14.815	41.68	26.87	25.66	.000	.000	.000
900	16.047	44.73	28.68	26.13	.000	.000	.000
1000	17.075	47.50	30.43	26.52	.000	.000	.000
1100	17.950	50.04	32.09	26.86	.000	.000	.000
1200	18.705	52.40	33.70	27.17	.000	.000	.000
1300	19.367	54.58	35.21	27.44	.000	.000	.000
1400	19.952	56.62	36.67	27.68	.000	.000	.000
1500	20.475	58.54	38.06	27.91	.000	.000	.000
1600	20.946	60.35	39.40	28.12	.000	.000	.000
1685	21.312	61.81	40.50	28.28	.000	.000	.000
1685	51.312	91.81	40.50	25.52	.000	.000	.000
1700	51.085	92.03	40.95	25.52	.000	.000	.000
1800	49.664	93.49	43.83	25.52	.000	.000	.000

MELTING POINT	1685 K	BOILING POINT	3553 K
ENTHALPY OF MELTING	50.551 kJ	ENTHALPY OF VAPORIZATION	392.840 kJ
$H_{298}^0 - H_0^0$	3.217 kJ	MOLAR VOLUME	1.2056 J/bar 12.056 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 31.778 + 5.3878 \times 10^{-4} T - 1.7864 \times 10^{-7} T^{0.5} - 1.4654 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1685 K)

REFERENCE 107 107

COMPILED  
4-10-76

SAMARIUM (REFERENCE STATE)

FORMULA WEIGHT 150.400

Sm: Alpha crystals (rhombohedral) 298.15 to 1190 K. Beta crystals (body-centered cubic) 1190 to melting point 1345 K. Liquid 1345 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>p</sub> <sup>0</sup> J/mol·K			
298.15	0.000	69.50	69.50	29.63	0.000	0.000	0.000
UNCERTAINTY		2.09	2.09				
400	7.900	78.59	70.69	33.20	.000	.000	.000
500	13.426	86.50	73.07	37.68	.000	.000	.000
600	17.745	93.66	75.91	40.75	.000	.000	.000
700	21.176	100.10	78.92	42.58	.000	.000	.000
800	23.924	105.86	81.94	43.66	.000	.000	.000
900	26.163	111.05	84.89	44.47	.000	.000	.000
1000	28.038	115.78	87.74	45.36	.000	.000	.000
1100	29.667	120.16	90.49	46.63	.000	.000	.000
1190	30.899	123.79	92.89	48.27	.000	.000	.000
1190	33.662	126.55	92.89	46.94	.000	.000	.000
1200	33.772	126.93	93.16	46.94	.000	.000	.000
1300	34.785	130.69	95.90	46.94	.000	.000	.000
1345	35.195	132.39	97.20	46.94	.000	.000	.000
1345	41.603	138.80	97.20	50.21	.000	.000	.000
1400	41.941	140.71	98.77	50.21	.000	.000	.000
1500	42.493	144.18	101.69	50.21	.000	.000	.000
1600	42.975	147.42	104.44	50.21	.000	.000	.000
1700	43.401	150.46	107.06	50.21	.000	.000	.000
1800	43.778	153.33	109.55	50.21	.000	.000	.000

MELTING POINT	1345 K	BOILING POINT	2064 K
ENTHALPY OF MELTING	8.619 kJ	ENTHALPY OF VAPORIZATION	166.405 kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	7.573 kJ	MOLAR VOLUME	1.9980 J/bar 19.980 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATIONS

$$C_p^0 = 4.0750 \times 10^{-2} - 0.23954 T + 7.9004 \times 10^{-5} T^2 - 6.5623 \times 10^{-8} T^{0.5} + 5.9178 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1190 K)

REFERENCE 107 107

COMPILED  
4-27-76

TiN (REFERENCE STATE)

FORMULA WEIGHT 118.690

Sn: Crystals 298.15 to melting point 505.1 K. Liquid 505 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	51.20	51.20	26.99	0.000	0.000	0.000
UNCERTAINTY		0.42	0.42				
400	7.102	59.39	52.29	28.83	.000	.000	.000
500	11.632	66.02	54.39	30.64	.000	.000	.000
505.1	11.897	67.13	55.23	30.73	.000	.000	.000
505.1	25.814	81.04	55.23	29.69	.000	.000	.000
600	26.260	85.24	58.98	28.82	.000	.000	.000
700	26.599	89.66	63.06	28.50	.000	.000	.000
800	26.831	93.46	66.63	28.45	.000	.000	.000
900	27.008	96.80	69.79	28.45	.000	.000	.000
1000	27.152	99.80	72.65	28.45	.000	.000	.000
1100	27.272	102.51	75.24	28.45	.000	.000	.000
1200	27.372	104.99	77.62	28.45	.000	.000	.000
1300	27.458	107.27	79.81	28.45	.000	.000	.000
1400	27.530	109.38	81.85	28.45	.000	.000	.000
1500	27.592	111.35	83.76	28.45	.000	.000	.000
1600	27.645	113.18	85.53	28.45	.000	.000	.000
1700	27.691	114.90	87.21	28.45	.000	.000	.000
1800	27.732	116.53	88.80	28.45	.000	.000	.000

MELTING POINT	505.1 K	BOILING POINT	2876 K
ENTHALPY OF MELTING	7.029 kJ	ENTHALPY OF VAPORIZATION	295.770 kJ
$H_{298}^0 - H_0^0$	6.322 kJ	MOLAR VOLUME	1.6289 J/bar 16.289 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 5.0767 \times 10^{-2} T - 2.3035 \times 10^{-5} T^2 + 2.5175 \times 10^2 T^{-0.5} - 6.0419 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 505.1 K)

REFERENCE 107 107

COMPILED  
4-10-76

STRONTIUM (REFERENCE STATE)

FORMULA WEIGHT 87.620

Sr: Alpha crystals (face-centered cubic) 298.15 to 828 K. Gamma crystals (body-centered cubic) 828 to melting point 1041 K. Liquid 1041 to boiling point 1652 K. Ideal monatomic gas 1652 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	55.40	55.40	29.18	0.000	0.000	0.000
UNCERTAINTY		0.17	0.17				
400	7.020	63.49	56.47	28.41	.000	.000	.000
500	11.468	70.01	58.54	30.12	.000	.000	.000
600	14.730	75.67	60.94	32.02	.000	.000	.000
700	17.353	80.76	63.41	34.22	.000	.000	.000
800	19.620	85.50	65.88	36.82	.000	.000	.000
828	19.970	86.83	66.86	37.63	.000	.000	.000
828	21.121	87.98	66.86	37.66	.000	.000	.000
900	22.444	90.83	68.39	37.66	.000	.000	.000
1000	23.966	94.79	70.82	37.66	.000	.000	.000
1041	24.503	96.44	71.93	37.66	.000	.000	.000
1041	32.381	104.31	71.93	35.15	.000	.000	.000
1100	32.529	106.12	73.59	35.15	.000	.000	.000
1200	32.747	109.18	76.43	35.15	.000	.000	.000
1300	32.932	111.99	79.06	35.15	.000	.000	.000
1400	33.089	114.59	81.50	35.15	.000	.000	.000
1500	33.227	117.02	83.79	35.15	.000	.000	.000
1600	33.346	119.29	85.94	35.15	.000	.000	.000
1652	33.403	120.41	87.00	35.15	.000	.000	.000
1652	116.317	203.31	87.00	20.82	.000	.000	.000
1700	113.621	203.81	90.19	20.82	.000	.000	.000
1800	108.468	205.01	96.54	20.82	.000	.000	.000

MELTING POINT	1041 K	BOILING POINT	1652 K
ENTHALPY OF MELTING	8.201 kJ	ENTHALPY OF VAPORIZATION	136.973 kJ
$H_{298}^0 - H_0^0$	6.360 kJ	MOLAR VOLUME	3.3921 J/bar 33.921 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 63.451 - 3.4824 \times 10^{-2} T + 3.2359 \times 10^{-5} T^2 - 5.6480 \times 10^2 T^{-0.5} \\ 3.1230 \times 10^5 T^{-2} \\ \text{(EQUATION VALID FROM 298 - 828 K)}$$

REFERENCE 107 124

COMPILED  
5-11-76

TANTALUM (REFERENCE STATE)

FORMULA WEIGHT 180.948

Ta: Body-centered cubic crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	41.51	41.51	25.36	0.000	0.000	0.000
UNCERTAINTY							
		0.17	0.17				
400	6.547	49.06	42.51	25.96	.000	.000	.000
500	10.464	54.89	44.43	26.28	.000	.000	.000
600	13.120	59.70	46.58	26.53	.000	.000	.000
700	15.051	63.81	48.76	26.75	.000	.000	.000
800	16.529	67.40	50.87	26.98	.000	.000	.000
900	17.703	70.59	52.89	27.22	.000	.000	.000
1000	18.667	73.47	54.80	27.47	.000	.000	.000
1100	19.479	76.10	56.62	27.74	.000	.000	.000
1200	20.180	78.53	58.35	28.03	.000	.000	.000
1300	20.795	80.78	59.98	28.34	.000	.000	.000
1400	21.346	82.90	61.55	28.68	.000	.000	.000
1500	21.847	84.89	63.04	29.03	.000	.000	.000
1600	22.307	86.77	64.46	29.41	.000	.000	.000
1700	22.737	88.57	65.83	29.82	.000	.000	.000
1800	23.142	90.28	67.14	30.24	.000	.000	.000

MELTING POINT	3287	K	BOILING POINT	5731	K
ENTHALPY OF MELTING	31.631	kJ	ENTHALPY OF VAPORIZATION	743.130	kJ
$H_{298}^0 - H_0^0$	5.636	kJ	MOLAR VOLUME	1.0851	J/bar cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS					

HEAT CAPACITY EQUATION

$$C_P^0 = 26.354 + 1.2092 \times 10^{-6} T^2 - 9.4252 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-17-76

## TERBIUM (REFERENCE STATE)

FORMULA WEIGHT 158.925

Tb: Alpha crystals (hexagonal close packed) 298.15 to 1560 K. Beta crystals (body-centered cubic) 1560 to melting point 1630 K. Liquid 1630 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	73.30	73.30	28.91	0.000	0.000	0.000
UNCERTAINTY		0.84	0.84				
400	7.225	81.63	74.40	28.15	.000	.000	.000
500	11.452	87.97	76.52	28.76	.000	.000	.000
600	14.428	93.31	78.88	29.90	.000	.000	.000
700	16.736	98.02	81.28	31.29	.000	.000	.000
800	18.650	102.30	83.65	32.81	.000	.000	.000
900	20.311	106.25	85.94	34.41	.000	.000	.000
1000	21.803	109.96	88.16	36.06	.000	.000	.000
1100	23.175	113.48	90.31	37.73	.000	.000	.000
1200	24.458	116.83	92.37	39.43	.000	.000	.000
1300	25.675	120.06	94.38	41.14	.000	.000	.000
1400	26.843	123.17	96.33	42.86	.000	.000	.000
1500	27.967	126.19	98.22	44.60	.000	.000	.000
1560	28.676	128.03	99.36	45.64	.000	.000	.000
1560	31.895	131.26	99.36	27.74	.000	.000	.000
1600	31.791	131.96	100.17	27.74	.000	.000	.000
1630	31.727	132.58	100.86	27.74	.000	.000	.000
1630	38.349	139.21	100.86	46.48	.000	.000	.000
1700	38.682	141.08	102.40	46.48	.000	.000	.000
1800	39.113	143.76	104.65	46.48	.000	.000	.000

MELTING POINT	1630	K	BOILING POINT	3496	K
ENTHALPY OF MELTING	10.795	kJ	ENTHALPY OF VAPORIZATION	330.890	kJ
$H_{298}^0 - H_0^0$	9.426	kJ	MOLAR VOLUME	1.9290 J/bar 19.290 $\text{cm}^3$	

## TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATION

$$C_P^0 = 17.894 + 1.7650 \times 10^{-2} T + 5.1149 \times 10^{-5} T^2$$

(EQUATION VALID FROM 298 - 1560 K)

REFERENCE 107 107

COMPILED  
7-29-76

TELLURIUM (REFERENCE STATE)

FORMULA WEIGHT 127.600

Te: Crystals 298.15 to melting point 723 K. Liquid 723 to boiling point  
1261 K. Ideal diatomic gas 1261 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	49.50	49.50	25.70	0.000	0.000	0.000
UNCERTAINTY		0.42	0.42				
400	6.830	57.37	50.54	27.95	.000	.000	.000
500	11.272	63.85	52.58	30.15	.000	.000	.000
600	14.602	69.54	54.94	32.36	.000	.000	.000
700	17.297	74.69	57.39	34.57	.000	.000	.000
723	17.866	76.22	58.36	35.07	.000	.000	.000
723	42.055	100.41	58.36	37.66	.000	.000	.000
800	41.631	103.83	62.20	37.66	.000	.000	.000
900	41.189	108.27	67.08	37.66	.000	.000	.000
1000	40.835	112.23	71.39	37.66	.000	.000	.000
1100	40.546	115.82	75.27	37.66	.000	.000	.000
1200	40.305	119.10	78.80	37.66	.000	.000	.000
1261	40.177	120.97	80.79	37.66	.000	.000	.000
1261	80.099	160.89	80.79	18.66	.000	.000	.000
1300	78.256	161.46	83.20	18.66	.000	.000	.000

MELTING POINT	723 K	BOILING POINT	1261 K
ENTHALPY OF MELTING	17.489 kJ	ENTHALPY OF VAPORIZATION	50.341 kJ
$H_{298}^0 - H_0^0$	6.121 kJ	MOLAR VOLUME	2.0476 J/bar 20.476 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 19.124 + 2.2061 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 723 K)

REFERENCE 107 107 COMPILED 8-06-76

## THORIUM (REFERENCE STATE)

FORMULA WEIGHT 232.038

Th: Alpha crystals (face-centered cubic) 298.15 to 1636 K. Beta crystals  
(body-centered cubic) 1636 to melting point 2028 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	53.39	53.39	27.32	0.000	0.000	0.000
UNCERTAINTY		0.84	0.84				
400	7.130	61.61	54.48	28.65	.000	.000	.000
500	11.560	68.14	56.58	29.92	.000	.000	.000
600	14.727	73.71	58.98	31.19	.000	.000	.000
700	17.169	78.61	61.44	32.46	.000	.000	.000
800	19.160	83.03	63.87	33.73	.000	.000	.000
900	20.849	87.07	66.22	35.00	.000	.000	.000
1000	22.328	90.83	68.50	36.27	.000	.000	.000
1100	23.654	94.34	70.69	37.55	.000	.000	.000
1200	24.864	97.66	72.80	38.82	.000	.000	.000
1300	25.987	100.82	74.83	40.09	.000	.000	.000
1400	27.040	103.84	76.80	41.37	.000	.000	.000
1500	28.037	106.74	78.70	42.64	.000	.000	.000
1600	28.990	109.53	80.54	43.92	.000	.000	.000
1636	29.304	110.53	81.27	44.38	.000	.000	.000
1636	30.997	112.27	81.27	46.02	.000	.000	.000
1700	31.562	113.95	82.39	46.02	.000	.000	.000
1800	32.366	116.58	84.21	46.02	.000	.000	.000

MELTING POINT	2028	K	BOILING POINT	5061	K
ENTHALPY OF MELTING	16.120	kJ	ENTHALPY OF VAPORIZATION	514.460	kJ
$H_{298}^0 - H_0^0$	6.510	kJ	MOLAR VOLUME	1.9788	J/bar
				19.788	cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATION

$$C_P^0 = 23.317 + 1.2793 \times 10^{-2} T + 5.4662 T^{-0.5} - 9.2289 \times 10^{-3} T^{-2}$$

(EQUATION VALID FROM 298 - 1636 K)

REFERENCE 107 107

COMPILED  
4-15-76



TITANIUM (REFERENCE STATE)

FORMULA WEIGHT 47.900

Ti: Alpha crystals (hexagonal close packed) 298.15 to 1155 K. Beta crystals (body-centered cubic) 1155 to melting point 1943 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	30.63	30.63	25.02	0.000	0.000	0.000
UNCERTAINTY		0.08	0.08				
400	6.545	38.18	31.63	26.35	.000	.000	.000
500	10.614	44.17	33.56	27.39	.000	.000	.000
600	13.492	49.25	35.76	28.37	.000	.000	.000
700	15.686	53.70	38.01	29.34	.000	.000	.000
800	17.454	57.68	40.23	30.32	.000	.000	.000
900	18.938	61.31	42.37	31.31	.000	.000	.000
1000	20.226	64.66	44.43	32.32	.000	.000	.000
1100	21.373	67.79	46.42	33.35	.000	.000	.000
1155	21.919	69.45	47.53	33.92	.000	.000	.000
1155	25.617	73.15	47.53	29.25	.000	.000	.000
1200	25.790	74.24	48.45	29.72	.000	.000	.000
1300	26.132	76.66	50.53	30.75	.000	.000	.000
1400	26.499	78.98	52.48	31.79	.000	.000	.000
1500	26.887	81.21	54.32	32.83	.000	.000	.000
1600	27.290	83.36	56.07	33.86	.000	.000	.000
1700	27.707	85.44	57.73	34.90	.000	.000	.000
1800	28.136	87.47	59.33	35.94	.000	.000	.000

MELTING POINT	1943 K	BOILING POINT	3562 K
ENTHALPY OF MELTING	15.447 kJ	ENTHALPY OF VAPORIZATION	421.031 kJ
$H_{298}^0 - H_0^0$	4.807 kJ	MOLAR VOLUME	1.0631 J/bar 10.631 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_p^0 = 17.208 + 1.1603 \times 10^{-2} T + 1.1826 \times 10^{-5} T^2 - 2.2609 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1155 K)

$$C_p^0 = 17.274 + 1.0368 \times 10^{-2} T$$

(EQUATION VALID FROM 1155 - 1800 K)

REFERENCE 107 107

COMPILED  
4-10-76

## THALLIUM (REFERENCE STATE)

FORMULA WEIGHT 204.370

Tl: Alpha crystals (hexagonal close packed) 298.15 to 507 K. Beta crystals (body-centered cubic) 507 to melting point 577 K. Liquid 577 K to 1744 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	64.18	64.18	26.33	0.000	0.000	0.000
UNCERTAINTY		0.21	0.21				
400	6.827	72.05	65.22	27.44	.000	.000	.000
500	11.134	78.37	67.24	29.45	.000	.000	.000
507	11.388	78.78	67.40	29.66	.000	.000	.000
507	12.131	79.54	67.40	32.01	.000	.000	.000
577	14.582	83.72	69.12	32.68	.000	.000	.000
577	21.761	90.88	69.12	29.71	.000	.000	.000
600	22.063	92.04	69.98	29.71	.000	.000	.000
700	23.156	96.62	73.46	29.71	.000	.000	.000
800	23.975	100.59	76.61	29.71	.000	.000	.000
900	24.611	104.09	79.48	29.71	.000	.000	.000
1000	25.121	107.22	82.10	29.71	.000	.000	.000
1100	25.538	110.05	84.51	29.71	.000	.000	.000
1200	25.885	112.64	86.76	29.71	.000	.000	.000
1300	26.179	115.01	88.83	29.71	.000	.000	.000
1400	26.431	117.22	90.79	29.71	.000	.000	.000
1500	26.649	119.26	92.61	29.71	.000	.000	.000
1600	26.841	121.18	94.34	29.71	.000	.000	.000
1700	27.009	122.98	95.97	29.71	.000	.000	.000
1744	27.077	123.77	96.70	29.71	.000	.000	.000
1744	121.200	217.90	96.70	22.05	.000	.000	.000
1800	118.115	218.56	100.44	22.05	.000	.000	.000

MELTING POINT	577 K	BOILING POINT	1744 K
ENTHALPY OF MELTING	4.142 kJ	ENTHALPY OF VAPORIZATION	164.151 kJ
$H_{298}^0 - H_0^0$	6.828 kJ	MOLAR VOLUME	1.7210 J/bar 17.210 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 30.850 - 2.8925 \times 10^{-2} T + 5.3134 \times 10^{-5} T^2 - 5.4964 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 507 K)

REFERENCE 107 107

COMPILED  
4-30-76

THULIUM (REFERENCE STATE)

FORMULA WEIGHT 168.934

T<sub>m</sub>: Hexagonal close packed crystals 298.15 to melting point 1818 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	74.01	74.01	27.03	0.000	0.000	0.000
UNCERTAINTY		0.00	0.00				
400	6.750	81.81	75.06	26.39	.000	.000	.000
500	10.730	87.75	77.02	26.97	.000	.000	.000
600	13.508	92.74	79.23	27.86	.000	.000	.000
700	15.627	97.11	81.48	28.81	.000	.000	.000
800	17.334	101.02	83.69	29.75	.000	.000	.000
900	18.767	104.58	85.81	30.65	.000	.000	.000
1000	19.996	107.85	87.85	31.51	.000	.000	.000
1100	21.080	110.89	89.81	32.33	.000	.000	.000
1200	22.050	113.74	91.69	33.10	.000	.000	.000
1300	22.929	116.42	93.49	33.85	.000	.000	.000
1400	23.736	118.95	95.21	34.56	.000	.000	.000
1500	24.480	121.36	96.88	35.25	.000	.000	.000
1600	25.174	123.66	98.49	35.92	.000	.000	.000
1700	25.825	125.85	100.02	36.56	.000	.000	.000
1800	26.439	127.96	101.52	37.19	.000	.000	.000

MELTING POINT	1818 K	BOILING POINT	2220 K
ENTHALPY OF MELTING	16.841 kJ	ENTHALPY OF VAPORIZATION	190.670 kJ
$H_{298}^0 - H_0^0$	7.397 kJ	MOLAR VOLUME	1.8126 J/bar 18.126 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 38.778 + 3.9669 \times 10^{-3} T - 3.8099 \times 10^{-2} T^{-0.5} + 8.1192 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
6-9-76

## URANIUM (REFERENCE STATE)

FORMULA WEIGHT 238.029

U: Alpha crystals (orthorhombic) 298.15 to 941 K. Beta crystals (tetragonal) 941 to 1048 K. Gamma crystals (body-centered cubic) 1048 to melting point 1405 K. Liquid 1405 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	50.29	50.29	27.68	0.000	0.000	0.000
UNCERTAINTY		0.13	0.13				
400	7.297	58.70	51.40	29.69	.000	.000	.000
500	12.000	65.56	53.56	32.00	.000	.000	.000
600	15.557	71.63	56.07	34.76	.000	.000	.000
700	18.527	77.23	58.70	38.01	.000	.000	.000
800	21.192	82.55	61.36	41.78	.000	.000	.000
900	23.716	87.71	63.99	46.09	.000	.000	.000
941	24.735	89.79	65.06	48.01	.000	.000	.000
941	27.701	92.76	65.06	45.67	.000	.000	.000
1000	28.596	95.38	66.78	42.93	.000	.000	.000
1048	30.608	98.88	68.27	42.93	.000	.000	.000
1048	33.792	102.06	68.27	38.28	.000	.000	.000
1100	34.005	103.79	69.79	38.28	.000	.000	.000
1200	34.361	107.12	72.76	38.28	.000	.000	.000
1300	34.662	110.19	75.53	38.28	.000	.000	.000
1400	34.921	113.02	78.10	38.28	.000	.000	.000
1405	34.933	113.36	78.43	38.28	.000	.000	.000
1405	40.996	119.42	78.43	47.91	.000	.000	.000
1500	41.434	122.36	80.93	47.91	.000	.000	.000
1600	41.839	125.45	83.61	47.91	.000	.000	.000
1700	42.195	128.35	86.15	47.91	.000	.000	.000
1800	42.513	131.09	88.58	47.91	.000	.000	.000

MELTING POINT	1405	K	BOILING POINT	4407	K
ENTHALPY OF MELTING	8.519	kJ	ENTHALPY OF VAPORIZATION	464.070	kJ
$H_{298}^0 - H_0^0$	6.364	kJ	MOLAR VOLUME	1.2497	J/bar 12.497 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 32.935 - 7.7083 \times 10^{-3} T + 2.8721 \times 10^{-5} T^2 - 95.207 T^{-0.5}$$

(EQUATION VALID FROM 298 - 941 K)

REFERENCE	107	107	COMPILED
			4-30-76

VANADIUM (REFERENCE STATE)

FORMULA WEIGHT 50.941

V: Body-centered cubic crystals 298.15 to melting point 2175

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	28.91	28.91	24.89	0.000	0.000	0.000
UNCERTAINTY							
		0.42	0.42				
400	6.515	36.42	29.90	26.09	.000	.000	.000
500	10.504	42.32	31.82	26.79	.000	.000	.000
600	13.272	47.26	33.99	27.42	.000	.000	.000
700	15.340	51.54	36.20	28.09	.000	.000	.000
800	16.979	55.34	38.36	28.83	.000	.000	.000
900	18.340	58.78	40.44	29.64	.000	.000	.000
1000	19.515	61.95	42.43	30.55	.000	.000	.000
1100	20.563	64.91	44.35	31.55	.000	.000	.000
1200	21.522	67.70	46.18	32.63	.000	.000	.000
1300	22.422	70.36	47.94	33.80	.000	.000	.000
1400	23.279	72.91	49.63	35.06	.000	.000	.000
1500	24.109	75.37	51.26	36.41	.000	.000	.000
1600	24.922	77.77	52.85	37.84	.000	.000	.000
1700	25.727	80.11	54.38	39.36	.000	.000	.000
1800	26.529	82.40	55.87	40.97	.000	.000	.000

MELTING POINT	2175	K	BOILING POINT	3682	K
ENTHALPY OF MELTING	20.928	kJ	ENTHALPY OF VAPORIZATION	451.893	kJ
$H_{298}^0 - H_0^0$	4.640	kJ	MOLAR VOLUME	0.8350 J/bar 8.350 cm <sup>3</sup>	

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 20.403 + 2.8000 \times 10^{-3} T + 3.9747 \times 10^{-6} T^2 + 1.1614 \times 10^{-9} T^3 - 2.9947 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-10-76

TUNGSTEN (REFERENCE STATE)

FORMULA WEIGHT 183.850

W: Body-centered cubic crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS		
					ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	32.64	32.64	24.26	0.000	0.000	0.000
UNCERTAINTY		0.42	0.42				
400	6.295	39.90	33.60	25.09	.000	.000	.000
500	10.108	45.56	35.45	25.60	.000	.000	.000
600	12.723	50.26	37.54	25.99	.000	.000	.000
700	14.646	54.29	39.64	26.34	.000	.000	.000
800	16.129	57.83	41.70	26.67	.000	.000	.000
900	17.318	60.99	43.67	26.99	.000	.000	.000
1000	18.301	63.85	45.55	27.31	.000	.000	.000
1100	19.134	66.47	47.34	27.62	.000	.000	.000
1200	19.854	68.89	49.04	27.94	.000	.000	.000
1300	20.488	71.14	50.65	28.26	.000	.000	.000
1400	21.056	73.24	52.18	28.59	.000	.000	.000
1500	21.569	75.23	53.66	28.92	.000	.000	.000
1600	22.039	77.10	55.06	29.26	.000	.000	.000
1700	22.474	78.89	56.42	29.60	.000	.000	.000
1800	22.879	80.59	57.71	29.95	.000	.000	.000

MELTING POINT	3680	K	BOILING POINT	5828	K
ENTHALPY OF MELTING	35.397	kJ	ENTHALPY OF VAPORIZATION	823.913	kJ
$H_{298}^0 - H_0^0$	4.979	kJ	MOLAR VOLUME	0.9545 J/bar 9.545 cm <sup>3</sup>	

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 24.843 + 2.2255 \times 10^{-3} T + 3.5044 \times 10^{-7} T^2 - 1.1153 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 107 107

COMPILED  
4-11-76

XENON (REFERENCE STATE)

FORMULA WEIGHT 131.300

Xe: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	169.68	169.68	20.79	0.000	0.000	0.000
UNCERTAINTY		0.02	0.02				
400	5.292	175.79	170.50	20.79	.000	.000	.000
500	8.392	180.43	172.04	20.79	.000	.000	.000
600	10.457	184.22	173.76	20.79	.000	.000	.000
700	11.933	187.42	175.49	20.79	.000	.000	.000
800	13.040	190.20	177.16	20.79	.000	.000	.000
900	13.900	192.64	178.74	20.79	.000	.000	.000
1000	14.589	194.83	180.24	20.79	.000	.000	.000
1100	15.152	196.82	181.67	20.79	.000	.000	.000
1200	15.622	198.62	183.00	20.79	.000	.000	.000
1300	16.019	200.29	184.27	20.79	.000	.000	.000
1400	16.359	201.83	185.47	20.79	.000	.000	.000
1500	16.655	203.26	186.61	20.79	.000	.000	.000
1600	16.912	204.60	187.69	20.79	.000	.000	.000
1700	17.141	205.86	188.72	20.79	.000	.000	.000
1800	17.343	207.05	189.71	20.79	.000	.000	.000

MELTING POINT	161.36 K	BOILING POINT	165.03 K
ENTHALPY OF MELTING	2.297 kJ	ENTHALPY OF VAPORIZATION	12.636 kJ
$H_{298}^0 - H_0^0$	6.197 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE 107 35 COMPILED 3-11-76

## YTTRIUM (REFERENCE STATE)

FORMULA WEIGHT 88.906

Y: Alpha crystals (hexagonal close packed) 298.15 to 1752 K. Beta crystals (body-centered cubic) 1752 to melting point 1799 K. Liquid 1799 to boiling point 3611 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>P</sub> <sup>o</sup> J/mol·K			
298.15	0.000	44.43	44.43	26.53	0.000	0.000	0.000
UNCERTAINTY		0.25	0.25				
400	6.825	52.30	45.47	27.19	.000	.000	.000
500	10.968	58.44	47.47	27.88	.000	.000	.000
600	13.845	63.59	49.74	28.57	.000	.000	.000
700	15.999	68.05	52.05	29.28	.000	.000	.000
800	17.704	72.00	54.30	30.00	.000	.000	.000
900	19.110	75.58	56.47	30.73	.000	.000	.000
1000	20.309	78.85	58.54	31.48	.000	.000	.000
1100	21.359	81.89	60.53	32.24	.000	.000	.000
1200	22.297	84.73	62.43	33.00	.000	.000	.000
1300	23.151	87.40	64.25	33.78	.000	.000	.000
1400	23.938	89.93	65.99	34.56	.000	.000	.000
1500	24.672	92.34	67.67	35.34	.000	.000	.000
1600	25.364	94.65	69.29	36.13	.000	.000	.000
1700	26.021	96.86	70.84	36.93	.000	.000	.000
1752	26.343	97.99	71.63	37.45	.000	.000	.000
1752	29.192	100.83	71.63	35.02	.000	.000	.000
1799	29.344	101.76	72.42	35.02	.000	.000	.000
1799	35.679	108.07	72.42	43.10	.000	.000	.000
1800	35.681	108.11	72.43	43.09	.000	.000	.000

MELTING POINT	1799 K	BOILING POINT	3611 K
ENTHALPY OF MELTING	11.397 kJ	ENTHALPY OF VAPORIZATION	363.340 kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	5.966 kJ	MOLAR VOLUME	1.5038 J/bar 15.038 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATION

$$C_P^o = 20.985 + 8.4202 \times 10^{-3} T + 68.561 T^{-0.5} - 9.4871 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1752 K)

REFERENCE 107 107

COMPILED  
4-26-76



YTTERBIUM (REFERENCE STATE)

FORMULA WEIGHT 173.040

Yb: Alpha crystals (face-centered cubic) 298.15 to 1033 K. Beta crystals (body-centered cubic) 1033 to melting point 1097 K. Liquid 1097 to boiling point 1465 K. Ideal monatomic gas 1465 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	59.83	59.83	26.72	0.000	0.000	0.000
UNCERTAINTY		0.17	0.17				
400	6.900	67.79	60.89	27.61	.000	.000	.000
500	11.312	74.24	62.93	31.02	.000	.000	.000
553	13.220	77.66	64.44	34.90	.000	.000	.000
553	13.349	77.79	64.44	29.68	.000	.000	.000
600	14.658	79.97	65.31	29.84	.000	.000	.000
700	16.859	84.60	67.74	30.31	.000	.000	.000
800	18.574	88.68	70.11	30.85	.000	.000	.000
900	19.968	92.35	72.38	31.40	.000	.000	.000
1000	21.138	95.68	74.54	31.92	.000	.000	.000
1033	21.487	96.73	75.25	32.05	.000	.000	.000
1033	23.180	98.45	75.25	36.11	.000	.000	.000
1097	23.937	100.62	76.69	36.11	.000	.000	.000
1097	30.917	107.61	76.69	36.78	.000	.000	.000
1100	30.928	107.67	76.74	36.78	.000	.000	.000
1200	31.416	110.87	79.45	36.78	.000	.000	.000
1300	31.828	113.81	81.98	36.78	.000	.000	.000
1400	32.182	116.54	84.36	36.78	.000	.000	.000

MELTING POINT	1097	K	BOILING POINT	1465	K
ENTHALPY OF MELTING	7.657	kJ	ENTHALPY OF VAPORIZATION	128.935	kJ
$H_{298}^0 - H_0^0$	6.711	kJ	MOLAR VOLUME	2.4830	J/bar
				24.830	cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATIONS

$$C_P^0 = 5.1202 \times 10^{-2} - 0.73984 T + 5.6939 \times 10^{-4} T^2 - 5.8564 \times 10^{-7} T^{0.5} + 2.1191 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 553 K)

$$C_P^0 = 2.7211 \times 10^{-2} T - 7.9838 \times 10^{-6} T^2 + 4.0139 \times 10^{-2} T^{-0.5}$$

(EQUATION VALID FROM 553 - 1033 K)

REFERENCE 107 107

COMPILED  
4-30-76

ZINC (REFERENCE STATE) FORMULA WEIGHT 65.380

Zn: Hexagonal close packed crystals 298.15 to melting point 692.7 K. Liquid  
692.7 to boiling point 1178 K. Ideal monatomic gas 1178 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	41.63	41.63	25.40	0.000	0.000	0.000
UNCERTAINTY		0.13	0.13				
400	6.575	49.21	42.63	26.29	.000	.000	.000
500	10.620	55.19	44.57	27.31	.000	.000	.000
600	13.495	60.27	46.78	28.46	.000	.000	.000
692.66	15.584	64.47	48.89	29.59	.000	.000	.000
692.66	26.155	75.04	48.89	31.38	.000	.000	.000
700	26.210	75.35	49.14	31.38	.000	.000	.000
800	26.856	79.54	52.68	31.38	.000	.000	.000
900	27.359	83.23	55.87	31.38	.000	.000	.000
1000	27.761	86.54	58.78	31.38	.000	.000	.000
1100	28.090	89.53	61.44	31.38	.000	.000	.000
1178	28.306	91.68	63.35	31.38	.000	.000	.000
1178	126.229	189.55	63.35	20.79	.000	.000	.000
1200	124.296	189.93	65.63	20.79	.000	.000	.000
1300	116.334	191.59	75.26	20.79	.000	.000	.000
1400	109.509	193.13	83.62	20.79	.000	.000	.000
1500	103.594	194.57	90.98	20.79	.000	.000	.000
1600	98.418	195.91	97.49	20.79	.000	.000	.000
1700	93.852	197.17	103.32	20.79	.000	.000	.000
1800	89.793	198.36	108.57	20.79	.000	.000	.000

MELTING POINT	692.66 K	BOILING POINT	1178 K
ENTHALPY OF MELTING	7.322 kJ	ENTHALPY OF VAPORIZATION	115.353 kJ
$H_{298}^0 - H_0^0$	5.657 kJ	MOLAR VOLUME	0.9162 J/bar 9.162 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.8012 \times 10^{-2} T - 5.4094 \times 10^{-6} T^2 + 3.4981 \times 10^{-9} T^3 - 2.4584 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 692.66 K)

REFERENCE 107 35

COMPILED  
4-10-76

ZIRCONIUM (REFERENCE STATE) FORMULA WEIGHT 91.220

Zr: Hexagonal close packed crystals 298.15 to 1136 K. Body-centered cubic  
 crystals 1136 to melting point 2125 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol
298.15	0.000	38.99	38.99	25.37	0.000	0.000	0.000
UNCERTAINTY		0.17	0.17				
400	6.742	46.76	40.02	27.33	.000	.000	.000
500	10.974	52.98	42.01	28.42	.000	.000	.000
600	13.960	58.24	44.28	29.34	.000	.000	.000
700	16.223	62.84	46.62	30.25	.000	.000	.000
800	18.034	66.94	48.91	31.18	.000	.000	.000
900	19.546	70.66	51.11	32.11	.000	.000	.000
1000	20.850	74.09	53.24	33.06	.000	.000	.000
1100	22.003	77.29	55.29	34.00	.000	.000	.000
1136	22.368	78.48	56.12	34.33	.000	.000	.000
1136	25.855	81.97	56.12	31.38	.000	.000	.000
1200	26.150	83.58	57.43	31.38	.000	.000	.000
1300	26.552	86.09	59.54	31.38	.000	.000	.000
1400	26.897	88.41	61.51	31.38	.000	.000	.000
1500	27.196	90.58	63.38	31.38	.000	.000	.000
1600	27.457	92.60	65.14	31.38	.000	.000	.000
1700	27.688	94.51	66.82	31.38	.000	.000	.000
1800	27.893	96.30	68.41	31.38	.000	.000	.000

MELTING POINT	2125 K	BOILING POINT	4682 K
ENTHALPY OF MELTING	16.895 kJ	ENTHALPY OF VAPORIZATION	582.045 kJ
$H_{298}^0 - H_0^0$	5.531 kJ	MOLAR VOLUME	1.4016 J/bar 14.016 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 2.2629 \times 10^{-2} T - 3.6247 \times 10^{-6} T^2 + 4.6723 \times 10^2 T^{-0.5} - 7.2106 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1136 K)

REFERENCE	107	107	COMPILED
			4-13-76

## METHANE (IDEAL GAS)

FORMULA WEIGHT 16.043

CH<sub>4</sub>: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	186.26	186.26	35.64	-74.810	-50.708	8.884
UNCERTAINTY		0.21	0.21		0.335	0.377	0.066
400	9.600	197.30	187.70	40.32	-77.940	-41.984	5.483
500	16.346	206.95	190.60	46.41	-80.792	-32.667	3.413
600	21.862	215.95	194.09	52.41	-83.285	-22.799	1.985
700	26.627	224.45	197.82	57.96	-85.404	-12.548	0.936
800	30.865	232.52	201.66	63.01	-87.174	-2.014	0.131
900	34.689	240.21	205.52	67.58	-88.630	8.723	-0.506
1000	38.192	247.55	209.36	71.70	-89.792	19.598	-1.024
1100	41.410	254.56	213.15	75.41	-90.704	30.592	-1.453
1200	44.384	261.27	216.89	78.74	-91.398	41.645	-1.813
1300	47.143	267.69	220.55	81.71	-91.902	52.750	-2.120
1400	49.707	273.84	224.13	84.34	-92.246	63.895	-2.384
1500	52.095	279.74	227.64	86.66	-92.455	75.051	-2.614
1600	54.320	285.40	231.08	88.67	-92.559	86.240	-2.815
1700	56.393	290.83	234.44	90.40	-92.581	97.393	-2.993
1800	58.323	296.04	237.72	91.84	-92.549	108.566	-3.151

MELTING POINT	90.60 K	BOILING POINT	111.70 K
ENTHALPY OF MELTING	0.937 kJ	ENTHALPY OF VAPORIZATION	8.318 kJ
$H_{298}^0 - H_0^0$	10.025 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 78.976 + 4.3186 \times 10^{-2} T - 1.0598 \times 10^{-5} T^2 - 1.3202 \times 10^{-8} T^3 + 1.8836 \times 10^{-11} T^4$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	262	262	COMPILED 7-26-76
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COHENITE

FORMULA WEIGHT 179.552

Fe<sub>3</sub>C: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	104.43	104.43	111.03	24.937	19.912	-3.489
UNCERTAINTY		3.35	3.35		1.339	1.715	0.300
400	31.025	137.24	106.22	112.31	28.332	18.852	-2.462
500	47.414	164.65	117.24	113.56	29.820	15.228	-1.591
600	58.543	185.47	126.93	114.82	30.494	12.234	-1.065
700	66.671	203.26	136.59	116.07	30.347	9.134	-0.682
800	72.924	218.84	145.92	117.32	29.177	6.165	-0.403
900	77.922	232.73	154.81	118.58	26.634	3.501	-0.203
1000	82.054	245.30	163.24	119.83	21.874	1.163	-0.061
1100	85.545	256.77	171.22	121.08	14.408	-0.477	0.023
1200	88.559	267.36	178.80	122.33	9.643	-1.750	0.076
1300	91.205	277.20	185.99	123.59	9.353	-2.781	0.112
1400	93.564	286.41	192.85	124.84	8.906	-3.739	0.140
1500	95.689	295.06	199.37	126.09	8.421	-4.566	0.159
1600	97.629	303.24	205.61	127.34	7.792	-5.438	0.178
1700	99.414	311.00	211.59	128.60	3.502	-6.130	0.188
1800	101.070	318.38	217.31	129.85	1.579	-6.523	-0.189

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	18.112 kJ	MOLAR VOLUME	2.3230 J/bar 23.230 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.0730 \times 10^{-2} + 1.2528 \times 10^{-2} T$$

(EQUATION VALID FROM 463 - 1800 K)

REFERENCE	115	108	108	COMPILED 7-24-76
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## AMMONIA (IDEAL GAS)

FORMULA WEIGHT 17.030

NH<sub>3</sub>: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	192.78	192.78	35.63	-45.940	-16.410	2.875
UNCERTAINTY		0.08	0.08		0.350	0.350	0.061
400	9.450	203.67	194.22	38.70	-48.086	-5.984	0.781
500	15.628	212.65	197.02	41.98	-49.905	4.760	-0.497
600	20.290	220.59	200.30	45.19	-51.430	15.841	-1.379
700	24.067	227.79	203.72	48.25	-52.684	27.155	-2.026
800	27.272	234.42	207.15	51.14	-53.698	38.630	-2.522
900	30.078	240.60	210.52	53.85	-54.497	50.236	-2.916
1000	32.581	246.41	213.83	56.37	-55.113	61.887	-3.233
1100	34.852	251.89	217.04	58.72	-55.561	73.622	-3.496
1200	36.932	257.10	220.17	60.88	-55.868	85.377	-3.716
1300	38.852	262.05	223.20	62.87	-56.052	97.147	-3.903
1400	40.636	266.78	226.14	64.68	-56.126	108.933	-4.064
1500	42.293	271.30	229.01	66.32	-56.116	120.719	-4.204
1600	43.841	275.62	231.78	67.78	-56.031	132.535	-4.327
1700	45.288	279.77	234.48	69.07	-55.884	144.307	-4.434
1800	46.641	283.75	237.11	70.19	-55.695	156.066	-4.529

MELTING POINT	195.36 K	BOILING POINT	239.68 K
ENTHALPY OF MELTING	5.657 kJ	ENTHALPY OF VAPORIZATION	23.351 kJ
$H_{298}^0 - H_0^0$	10.046 kJ	MOLAR VOLUME	2478.92 J/bar 24789.2 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 29.735 + 3.9119 \times 10^{-2} T - 8.2274 \times 10^{-6} T^2 - 1.4378 \times 10^{-9} T^3 + 2.9243 \times 10^{-13} T^4$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	35	215	COMPILED
		215		7-26-76

ACANTHITE (ARGENTITE)

FORMULA WEIGHT 247.796

Ag<sub>2</sub>S: Monoclinic crystals 298.15 to 452 K. Cubic crystals (argentite) 452 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	142.84	142.84	75.32	-32.346	-40.080	7.022
UNCERTAINTY		0.42	0.42		0.879	0.837	0.147
400	20.605	166.52	145.92	86.57	-33.976	-42.485	5.548
452	27.544	177.66	150.12	92.31	-34.633	-44.140	5.101
452	37.983	188.11	150.12	90.54	-29.915	-44.140	5.101
500	43.012	196.02	153.01	90.54	-29.857	-44.995	4.701
600	50.905	212.50	161.60	90.54	-29.736	-48.082	4.186
700	56.544	226.44	169.89	90.54	-29.469	-51.142	3.816
800	60.825	238.57	177.74	90.54	-83.805	-59.823	3.906
900	64.108	249.20	185.09	90.54	-82.327	-56.838	3.299
1000	66.777	257.90	191.12	90.54	-80.980	-53.216	2.780

MELTING POINT	1061	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>		kJ	MOLAR VOLUME	3.4190 J/bar 34.190 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILVER..... M. P. 1234 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

REFERENCE	115	80	73	COMPILED 7-24-76
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## CHALCOCITE

FORMULA WEIGHT 159.152

$\text{Cu}_2\text{S}$ : Orthorhombic crystals 298.15 to 376 K. Hexagonal crystals 376 to 623 K. Cubic crystals 623 to melting point 1403 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	120.75	120.75	76.32	-80.115	-86.868	15.219
UNCERTAINTY		2.09	2.09		1.255	1.423	0.249
376	16.914	139.70	122.80	81.69	-82.216	-88.660	12.317
376	27.151	149.96	122.80	97.28	-78.366	-88.660	12.317
400	31.380	155.98	124.60	97.28	-77.297	-89.269	11.657
500	44.518	177.61	133.09	97.28	-76.675	-92.269	9.639
600	53.347	195.39	142.05	97.28	-75.816	-95.524	8.316
623	54.976	199.05	144.08	97.28	-75.618	-96.294	8.073
623	56.316	200.40	144.68	85.02	-74.784	-96.294	8.073
700	59.473	210.29	150.82	85.02	-74.926	-98.904	7.380
800	62.655	221.67	159.01	85.02	-129.768	-107.896	7.045
900	65.131	231.63	166.49	85.02	-128.693	-105.138	6.102
1000	67.111	240.62	173.51	85.02	-127.713	-102.631	5.361
1100	68.770	248.74	179.97	85.02	-126.775	-100.148	4.756
1200	70.117	256.14	186.03	85.02	-125.959	-97.782	4.256
1300	71.257	262.92	191.67	85.02	-125.221	-95.430	3.834
1400	72.234	269.20	196.96	85.02	-151.146	-92.571	3.454

MELTING POINT	1403	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.7475 J/bar 27.475 $\text{cm}^3$

## TRANSITIONS IN REFERENCE STATE ELEMENTS

COPPER..... M. P. 1357 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

REFERENCE	115	120	26	COMPILED
		266	219	7-24-76



CHALCOPYRITE

FORMULA WEIGHT 183.513

CuFeS<sub>2</sub>: Alpha crystals 298.15 to 830 K. Beta crystals 830 to 930 K. Gamma crystals 930 to 1200 K.

TEMP. K					FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0 - S_{298}^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $f$
298.15	0.000	0.00	---	95.77	---	---	---
UNCERTAINTY							
400	26.150	30.10	---	106.26	---	---	---
500	42.442	54.11	---	109.15	---	---	---
600	53.952	74.42	---	114.53	---	---	---
700	63.221	92.72	---	123.84	---	---	---
800	71.574	110.07	---	136.83	---	---	---
830	72.769	115.27	---	141.37	---	---	---
830	83.089	125.59	---	108.73	---	---	---
900	91.478	139.80	---	203.75	---	---	---
930	95.757	148.27	---	244.48	---	---	---
930	96.076	148.59	---	172.49	---	---	---
1000	101.425	160.10	---	172.49	---	---	---
1100	107.885	176.54	---	172.49	---	---	---
1200	113.269	191.55	---	172.49	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	J/bar

TRANSITIONS IN REFERENCE STATE ELEMENTS

COPPER..... M. P. 1357 K.

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = -5.8753 \times 10^2 + 0.37073 T + 1.2750 \times 10^4 T^{-0.5} - 1.4721 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 298 - 830 K)

$$C_P^0 = -1.0180 \times 10^3 + 1.3575 T$$

(EQUATION VALID FROM 830 - 930 K)

BORNITE

FORMULA WEIGHT 501.817

$\text{Cu}_3\text{FeS}_4$ : Alpha crystals 298.15 to 485 K. Beta crystals 485 to 540 K. Gamma crystals 540 to 1200 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$\frac{S_T^0}{S_{298}^0} -$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log f
298.15	0.000	0.00	---	---	---	---	---
UNCERTAINTY							
		0.00					
400	64.850	74.68	---	263.38	---	---	---
485	100.847	126.59	---	277.11	---	---	---
485	113.330	139.07	---	357.74	---	---	---
500	120.734	150.20	---	372.91	---	---	---
540	140.912	180.65	---	653.36	---	---	---
540	140.912	180.65	---	342.53	---	---	---
600	160.403	215.97	---	332.53	---	---	---
700	184.346	266.55	---	324.97	---	---	---
800	201.822	309.84	---	324.17	---	---	---
900	215.567	348.17	---	327.30	---	---	---
1000	226.999	382.93	---	332.87	---	---	---
1100	236.940	414.98	---	340.04	---	---	---
1200	245.870	444.91	---	348.30	---	---	---

MELTING POINT

K

BOILING POINT

K

ENTHALPY OF MELTING

kJ

ENTHALPY OF VAPORIZATION

kJ

 $H_{298}^0 - H_0^0$ 

kJ

MOLAR VOLUME

J/bar

TRANSITIONS IN REFERENCE STATE ELEMENTS

COPPER..... M. P. 1357 K.

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = -1.3274 \times 10^2 + 1.0113 T$$

(EQUATION VALID FROM 485 - 540 K)

$$C_P^0 = 1.8971 \times 10^2 + 0.11703 T + 2.6135 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 540 - 1200 K)

REFERENCE 209

COMPILED

8- 4-76

TROILITE

FORMULA WEIGHT 87.907

FeS: Alpha crystals 298.15 to 411 K. Beta crystals 411 to Curie point 598 K.  
Gamma crystals 598 to melting point 1468 K. Liquid 1468 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	60.33	60.33	50.50	-100.960	-101.333	17.753
UNCERTAINTY		0.17	0.17		1.464	1.506	0.264
400	15.375	77.94	62.57	65.90	-102.115	-101.283	13.226
411	16.580	79.85	63.27	67.56	-102.279	-101.340	12.879
411	21.517	84.79	63.27	76.94	-100.250	-101.340	12.879
500	31.464	99.78	68.32	76.94	-99.282	-101.576	10.612
598	37.440	112.04	74.60	76.94	-98.680	-102.140	8.922
598	39.058	113.66	74.60	57.00	-98.178	-102.140	8.922
600	39.120	113.84	74.72	57.02	-98.194	-102.152	8.893
700	41.960	122.92	80.96	58.02	-98.931	-102.744	7.667
800	44.089	130.79	86.70	59.01	-154.511	-108.772	7.102
900	45.746	137.73	91.99	60.01	-154.544	-102.980	5.977
1000	47.070	143.97	96.90	61.00	-155.344	-97.235	5.079
1100	48.230	149.66	101.43	62.00	-156.988	-91.315	4.336
1200	49.337	155.01	105.68	62.99	-157.590	-85.358	3.716
1300	50.465	160.16	109.69	63.99	-156.482	-79.444	3.192
1400	51.583	165.06	113.47	64.99	-155.255	-73.573	2.745
1468	52.289	168.30	116.01	65.66	-154.379	-69.562	2.475
1468	74.320	190.33	116.01	71.13	-122.037	-69.562	2.475
1500	74.252	191.79	117.54	71.13	-121.525	-68.477	2.385
1600	74.057	196.35	122.30	71.13	-119.926	-64.950	2.120
1700	73.885	200.66	126.78	71.13	-119.587	-61.515	1.890
1800	73.731	204.72	130.99	71.13	-118.500	-58.088	1.686

MELTING POINT	1468	K	BOILING POINT	K
ENTHALPY OF MELTING	32.342	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	1.8200 J/bar 18.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.  
SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 51.045 + 9.9579 \times 10^{-3} T$$

(EQUATION VALID FROM 598 - 1468 K)

REFERENCE	39	82	220	COMPILED
			2	7-24-76

PYRITE

FORMULA WEIGHT 119.967

FeS<sub>2</sub>: Crystals 298.15 to 1000 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	52.93	52.93	62.17	-171.544	-160.229	28.072
UNCERTAINTY		0.13	0.13		1.674	1.715	0.300
400	16.875	72.37	55.49	69.15	-176.747	-155.650	20.326
500	27.644	88.13	60.49	71.95	-180.349	-149.844	15.654
600	35.197	101.42	66.22	73.92	-183.303	-143.551	12.497
700	40.869	112.97	72.10	75.90	-185.781	-136.711	10.202
800	45.381	123.24	77.86	78.10	-297.402	-140.641	9.183
900	49.156	132.58	83.42	80.57	-297.233	-120.936	7.019
1000	52.427	141.21	88.78	83.29	-297.590	-101.339	5.293

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	9.632 kJ	MOLAR VOLUME	2.3940 J/bar 23.940 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.  
SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = -20.319 + 5.0299 \times 10^{-2} T + 1.7870 \times 10^{-3} T^2 - 3.2002 \times 10^{-6} T^3$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	39	80	255	COMPILED
	39			7-24-76

MARCASITE

FORMULA WEIGHT 119.967

FeS<sub>2</sub>: Crystals 298.15 to 700 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
					kJ/mol	kJ/mol	
298.15	0.000	53.89	53.89	62.43	-169.450	-158.421	27.755
UNCERTAINTY		0.11	0.11		2.090	2.090	0.366
400	16.850	73.29	56.44	69.18	-174.663	-153.934	20.102
500	27.680	89.12	61.44	72.46	-178.237	-148.227	15.485
600	35.323	102.52	67.20	74.58	-181.133	-142.041	12.366
700	41.093	114.19	73.10	77.04	-183.530	-135.314	10.097

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.4580 J/bar 24.580 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.  
SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -3.3463 \times 10^2 + 39.069 T^{0.5} - 1.1236 T + 3.0974 \times 10^{-4} T^2 + 8.9245 \times 10^{-7} T^{-1}$$

(EQUATION VALID FROM 298 - 700 K)

REFERENCE	81	81	81	COMPILED 7-24-76
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## HYDROGEN SULFIDE (IDEAL GAS)

FORMULA WEIGHT 34.076

H<sub>2</sub>S: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS		
					ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	205.80	205.80	34.19	-20.627	-33.543	5.877
UNCERTAINTY		0.21	0.21		0.628	0.669	0.117
400	8.850	216.01	207.16	35.48	-24.698	-37.375	4.881
500	14.346	224.10	209.75	37.21	-27.914	-40.118	4.191
600	18.310	231.05	212.74	39.05	-30.626	-42.346	3.687
700	21.401	237.21	215.81	40.85	-32.896	-44.100	3.291
800	23.941	242.77	218.83	42.57	-89.515	-51.108	3.337
900	26.100	247.88	221.78	44.20	-89.986	-46.230	2.683
1000	27.989	252.62	224.63	45.72	-90.338	-41.354	2.160
1100	29.665	257.04	227.37	47.12	-90.588	-36.441	1.730
1200	31.174	261.20	230.03	48.40	-90.746	-31.508	1.372
1300	32.545	265.12	232.57	49.57	-90.826	-26.569	1.068
1400	33.800	268.83	235.03	50.62	-90.845	-21.625	0.807
1500	34.952	272.36	237.41	51.54	-90.814	-16.695	0.581
1600	36.014	275.71	239.70	52.34	-90.739	-11.740	0.383
1700	36.996	278.91	241.91	53.03	-90.636	-6.821	0.210
1800	37.903	281.95	244.05	53.59	-90.518	-1.888	0.055

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	9.962 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 26.356 + 2.6497 \times 10^{-2} T - 6.0244 \times 10^{-6} T^2 - 43.559 T^{-0.5}$$

$$+ 2.6599 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	262	262	COMPILED 7-29-76
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ALABANDITE FORMULA WEIGHT 86.998

MnS: Crystals 298.15 to melting point 1803 K.

TEMP. K					FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	78.20	78.20	49.96	-213.865	-218.155	38.220
UNCERTAINTY		1.67	1.67		0.837	1.004	0.176
-----							
400	12.850	93.02	80.17	51.07	-216.151	-219.320	28.640
500	20.608	104.54	83.93	52.12	-217.836	-219.870	22.970
600	25.922	114.11	88.19	52.81	-219.289	-220.191	19.169
700	29.796	122.29	92.49	53.23	-220.586	-220.219	16.433
-----							
800	32.745	129.41	96.66	53.53	-276.509	-225.623	14.732
900	35.067	135.74	100.67	53.82	-276.535	-219.225	12.724
-----							
1000	36.963	141.42	104.46	54.19	-278.881	-212.797	11.115
-----							
1100	38.552	146.61	108.06	54.71	-279.081	-206.189	9.791
1200	39.927	151.40	111.47	55.42	-279.265	-199.543	8.686
1300	41.153	155.87	114.72	56.36	-279.415	-192.890	7.750
-----							
1400	42.279	160.09	117.81	57.58	-281.792	-186.168	6.946
-----							
1500	43.350	164.12	120.77	59.08	-284.251	-179.218	6.241
-----							
1600	44.387	167.98	123.59	60.88	-296.791	-171.519	5.600
1700	45.419	171.74	126.32	63.01	-297.079	-163.692	5.030
1800	46.464	175.41	128.95	65.48	-297.143	-155.845	4.523

MELTING POINT	1803	K	BOILING POINT	K
ENTHALPY OF MELTING	26.108	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.1460 J/bar 21.460 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.  
SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.3529 \times 10^2 - 5.7749 \times 10^{-2} T + 2.0865 \times 10^{-5} T^2 - 1.4352 \times 10^3 T^{-0.8}$$

$$1.1688 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	39	120	2	COMPILED
			49	7-26-76

## MOLYBDENITE

FORMULA WEIGHT 160.060

MoS<sub>2</sub>: Crystals 298.15 to 1200 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		Log K <sub>f</sub>
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T	S <sub>T</sub> <sup>o</sup>	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T	C <sub>P</sub> <sup>o</sup>	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	
298.15	0.000	62.57	62.57	63.55	-275.300	-266.454	46.681
UNCERTAINTY		0.21	0.21		5.000	5.000	0.880
400	16.850	81.99	65.14	68.48	-280.360	-262.734	34.310
500	27.520	97.64	70.12	71.61	-283.735	-257.838	26.937
600	35.062	110.90	75.84	73.80	-286.262	-252.504	21.983
700	40.714	122.40	81.69	75.38	-288.122	-246.683	18.408
800	45.126	132.55	87.42	76.57	-398.910	-251.761	16.438
900	48.678	141.62	92.94	77.47	-397.628	-233.346	13.543
1000	51.588	149.82	98.23	78.15	-396.351	-215.163	11.239
1100	54.029	157.29	103.26	78.68	-395.080	-197.113	9.360
1200	56.101	164.16	108.06	79.07	-393.828	-179.172	7.799

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	kJ	MOLAR VOLUME	3.2020 J/bar 32.020 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MOLYBDENUM. H. P. 2890 K.

SULFUR..... ORTHO-MONO 368.54, H. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^o = 1.0453 \times 10^2 - 4.8122 \times 10^{-3} T - 6.8169 \times 10^2 T^{-0.5} - 6.2906 \times 10^3 T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	61	165	286	COMPILED 03-15-79
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MILLERITE

FORMULA WEIGHT 90.760

NiS: Crystals 298.15 to 600 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	66.11	66.11	46.69	-84.868	-86.192	15.101
UNCERTAINTY		4.18	4.18		4.184	4.393	0.770
400	12.237	80.21	67.97	49.41	-87.406	-86.299	11.270
500	19.916	91.51	71.59	52.09	-89.225	-85.767	8.960
600	25.522	101.26	75.73	54.77	-90.739	-84.978	7.398

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
$H_{298}^0 - H_0^0$	KJ	MOLAR VOLUME	1.6890 J/bar 16.890 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

- NICKEL..... CURIE P. 631, M. P. 1726 K.
- SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 38.702 + 2.6778 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 600 K)

REFERENCE	115	80	231	COMPILED
		274		7-24-76

GALENA

FORMULA WEIGHT 239.260

PbS: Crystals 298.15 to melting point 1385 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	91.38	91.38	49.50	-97.709	-96.075	16.832
UNCERTAINTY		1.25	1.25		0.962	0.837	0.147
400	12.970	106.36	93.39	51.16	-99.918	-95.230	12.436
500	20.502	117.66	97.15	52.80	-101.566	-93.823	9.802
600	25.872	127.24	101.37	54.44	-102.777	-92.187	8.026
700	30.124	135.81	105.69	56.08	-108.387	-89.543	6.682
800	33.629	143.60	109.97	57.72	-163.431	-92.389	6.032
900	36.633	150.71	114.08	59.36	-162.182	-83.505	4.847

MELTING POINT	1385	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	3.1490 J/bar 31.490 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

LEAD..... M. P. 600.6, B. P. 2021 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 44.601 + 1.6401 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	115	120	245	COMPILED
			144	7-24-76

HERZENBERGITE

FORMULA WEIGHT 150.750

Sns: Alpha crystals 298.15 to 875 K. Beta crystals 875 to melting point  
1153 K. Liquid 1153 to 1300 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	76.82	76.82	49.25	-106.541	-104.698	18.343
UNCERTAINTY		0.84	0.84		1.464	1.506	0.264
400	12.800	91.59	78.79	50.87	-108.910	-103.755	13.549
500	20.524	103.05	82.53	52.02	-110.668	-102.212	10.678
600	25.962	112.74	86.78	54.51	-118.891	-99.135	8.630
700	30.303	121.42	91.12	58.40	-119.450	-95.766	7.146
800	34.124	129.54	95.42	63.50	-174.048	-97.930	6.394
875	36.416	135.12	98.70	67.97	-172.985	-90.640	5.411
875	37.303	136.01	98.70	53.28	-172.209	-90.640	5.411
900	37.811	137.47	99.66	54.04	-171.992	-88.501	5.136
1000	39.588	143.32	103.73	57.07	-171.124	-79.260	4.140
1100	41.315	148.90	107.58	60.11	-169.966	-70.135	3.330
1153	42.004	151.74	109.74	61.72	-169.474	-65.172	2.953
1153	69.401	179.14	109.74	75.61	-137.885	-65.172	2.953
1200	69.644	181.98	112.34	75.61	-136.545	-62.415	2.717
1300	70.103	188.03	117.93	75.61	-133.694	-56.347	2.264

MELTING POINT	1153 K	BOILING POINT	K
ENTHALPY OF MELTING	31.589 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.9010 J/bar 29.010 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

TIN..... M. P. 505 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = -1.5593 \times 10^{-2} + 0.12193 T + 3.6041 \times 10^{-5} T^2 - 3.5476 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 875 K)

$$C_P^0 = 26.722 + 3.0352 \times 10^{-2} T$$

(EQUATION VALID FROM 875 - 1153 K)

REFERENCE	192	120	220	COMPILED 7-24-76
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## STANNIC SULFIDE

FORMULA WEIGHT 182.810

SnS<sub>2</sub>: Crystals 298.15 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	87.45	87.45	70.12	---	---	---
UNCERTAINTY		0.18	0.18				
400	18.125	108.36	90.23	72.05	---	---	---
500	29.058	124.59	95.53	73.53	---	---	---
600	36.603	138.14	101.54	75.19	---	---	---
700	42.253	149.87	107.62	77.14	---	---	---
800	46.747	160.31	113.56	79.33	---	---	---
900	50.500	169.79	119.29	81.74	---	---	---
1000	53.752	178.54	124.79	84.33	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.0960 J/bar 40.960 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

TIN..... M. P. 505 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 20.042 + 3.8228 \times 10^{-2} T + 8.5441 \times 10^{-5} T^2 - 9.6017 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE 192 120

COMPILED  
7-24-76

SPHALERITE FORMULA WEIGHT 97.440

ZnS: Cubic crystals 298.15 to 1200 K. Wurtzite is the stable phase of ZnS above 1293 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	58.66	58.66	45.76	-206.900	-202.496	35.477
UNCERTAINTY		0.13	0.13		1.700	1.780	0.312
400	12.000	72.49	60.49	48.30	-209.378	-200.655	26.203
500	19.432	83.46	64.03	49.93	-211.067	-198.231	20.709
600	24.618	92.67	68.05	51.11	-212.397	-195.581	17.027
700	28.471	100.62	72.15	52.04	-220.819	-192.592	14.371
800	31.466	107.62	76.15	52.79	-276.553	-194.035	12.669
900	33.867	113.87	80.00	53.42	-276.217	-183.699	10.662
1000	35.853	119.53	83.68	53.96	-275.827	-173.433	9.059
1100	37.521	124.70	87.18	54.43	-275.399	-163.226	7.751
1200	38.948	129.45	90.50	54.85	-390.047	-150.953	6.571
1300	40.186	133.86	93.67	55.23	-388.484	-131.100	5.268

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.3830 J/bar 23.830 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ZINC..... M. P. 692.7, B. P. 1178 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 61.506 + 7.6314 \times 10^{-4} T - 2.6035 \times 10^{-2} T^{-0.5} - 7.9631 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE 208 120 2 COMPILED 7-24-76

## WURTZITE

FORMULA WEIGHT 97.440

ZnS: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	58.84	58.84	45.88	-194.570	-190.220	33.326
UNCERTAINTY		0.12	0.12		1.500	1.520	0.266
400	12.100	72.78	60.68	48.71	-197.008	-188.401	24.603
500	19.570	83.81	64.24	50.13	-198.668	-186.007	19.432
600	24.745	93.04	68.30	51.08	-199.991	-183.397	15.966
700	28.563	100.97	72.41	51.85	-208.425	-180.443	13.465
800	31.519	107.94	76.42	52.54	-264.181	-181.919	11.878
900	33.889	114.17	80.28	53.20	-263.867	-171.619	9.961
1000	35.855	119.81	83.95	53.85	-263.495	-161.381	8.430
1100	37.520	124.97	87.45	54.50	-263.070	-151.194	7.180
1200	38.962	129.74	90.78	55.14	-377.701	-138.955	6.049
1300	40.232	134.18	93.95	55.79	-376.095	-119.127	4.787

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.3846 J/bar 23.846 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

ZINC..... M. P. 692.7, B. P. 1178 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 41.906 + 7.6193 \times 10^{-3} T + 1.5767 \times 10^{-5} T^2 - 6.6034 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	208	248	215	COMPILED
			2	7-24-76

CORUNDUM

FORMULA WEIGHT 101.962

Al<sub>2</sub>O<sub>3</sub>: (Corundum), crystals 298.15 to melting point 2345 K.

TEMP.	FORMATION FROM THE ELEMENTS				ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	S <sub>T</sub> <sup>0</sup>	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	C <sub>P</sub> <sup>0</sup>			
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	50.92	50.92	79.01	-1675.700	-1582.228	277.201
UNCERTAINTY		0.10	0.10		1.300	1.320	0.231
400	22.575	76.85	54.27	96.39	-1676.304	-1550.162	202.431
500	38.372	99.47	61.10	105.95	-1675.984	-1518.654	158.653
600	50.187	119.38	69.19	112.19	-1675.264	-1487.257	129.478
700	59.377	137.02	77.64	116.65	-1674.404	-1455.990	108.648
800	66.756	152.83	86.07	120.04	-1673.565	-1424.841	93.033
900	72.833	167.13	94.30	122.73	-1672.865	-1393.793	80.894
1000	77.935	180.18	102.25	124.94	-1693.698	-1361.288	71.107
1100	82.294	192.17	109.88	126.79	-1692.719	-1328.080	63.066
1200	86.070	203.28	117.21	128.38	-1691.635	-1294.993	56.370
1300	89.378	213.61	124.23	129.77	-1690.457	-1261.964	50.707
1400	92.307	223.27	130.96	130.99	-1689.203	-1229.065	45.857
1500	94.924	232.34	137.42	132.08	-1687.872	-1196.232	41.657
1600	97.277	240.90	143.62	133.07	-1686.481	-1163.513	37.985
1700	99.409	249.00	149.59	133.96	-1685.029	-1130.906	34.749
1800	101.352	256.68	155.33	134.78	-1683.527	-1098.329	31.873

MELTING POINT	2345	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	10.016	kJ	MOLAR VOLUME	2.5575 J/bar 25.575 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.5736 \times 10^{-2} + 7.1899 \times 10^{-4} T - 9.8804 \times 10^{-7} T^{0.5} - 1.8969 \times 10^{-9} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	285	50	35	COMPILED
	50	66	159	7-21-76

## ALUMINUM OXIDE (GAMMA)

FORMULA WEIGHT 101.962

Al<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	59.83	59.83	79.02	-1653.517	-1562.702	273.780
UNCERTAINTY		6.28	6.28		1.260	1.300	0.228
400	22.600	85.79	63.19	96.49	-1654.111	-1531.545	200.000
500	38.406	108.43	70.02	106.01	-1653.784	-1500.934	156.802
600	50.222	128.34	78.12	112.20	-1653.060	-1470.429	128.013
700	59.407	145.98	86.57	116.62	-1652.200	-1440.058	107.459
800	66.777	161.78	95.00	119.99	-1651.365	-1409.801	92.051
900	72.844	176.08	103.24	122.67	-1650.672	-1379.655	80.073
1000	77.940	189.12	111.18	124.89	-1671.510	-1348.040	70.415
1100	82.295	201.11	118.81	126.76	-1670.534	-1315.729	62.479
1200	86.070	212.21	126.14	128.38	-1669.452	-1283.526	55.871
1300	89.380	222.54	133.16	129.81	-1668.272	-1251.388	50.282
1400	92.314	232.21	139.90	131.08	-1667.010	-1219.388	45.496
1500	94.937	241.29	146.35	132.23	-1665.670	-1187.455	41.351
1600	97.300	249.86	152.56	133.27	-1664.262	-1155.630	37.728
1700	99.445	257.97	158.53	134.23	-1662.786	-1123.912	34.534
1800	101.402	265.67	164.27	135.12	-1661.254	-1092.238	31.696

MELTING POINT	2291	K	BOILING POINT	K
ENTHALPY OF MELTING	94.140	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 1.5343 \times 10^2 + 1.9681 \times 10^{-3} T - 9.0063 \times 10^{-2} T^{-0.5} - 2.0307 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	32	32	32	COMPILED
				7-27-76



BOEHMITE FORMULA WEIGHT 59.989

AlO(OH): Crystals 298.15 to 500 K.

TEMP.					FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	48.45	48.45	65.63	-993.054	-918.400	160.900
UNCERTAINTY		0.21	0.21		2.110	2.090	0.366
400	16.297	67.19	50.90	67.43	-993.589	-892.723	116.583
500	28.660	84.54	55.88	69.18	-992.924	-867.565	90.640

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	8.828 kJ	MOLAR VOLUME	1.9535 J/bar 19.535 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 60.396 + 1.7573 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 500 K)

REFERENCE	115	120	94	COMPILED
			216	7-14-77

GIBBSITE FORMULA WEIGHT 78.004

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Al(OH)<sub>3</sub>: Crystals 298.15 to 480 K. Gibbsite decomposes above 480 K.

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TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	68.44	68.44	91.70	-1293.128	-1154.889	202.333
UNCERTAINTY		0.14	0.14		1.192	1.213	0.213
400	26.467	98.83	72.36	115.10	-1294.070	-1106.856	144.543

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	12.719 kJ	MOLAR VOLUME	3.1956 J/bar 31.956 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

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REFERENCE	95	95	93	COMPILED
				7-24-76

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BORIC OXIDE

FORMULA WEIGHT 69.618

B<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to melting point 723 K. Liquid 723 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	53.97	53.97	62.68	-1273.500	-1194.325	209.242
UNCERTAINTY		0.03	0.03		1.400	1.715	0.300
400	17.475	74.06	57.28	75.28	-1273.766	-1167.236	152.426
500	30.358	92.27	61.91	88.20	-1273.595	-1140.605	119.159
600	40.960	109.37	68.41	99.43	-1272.874	-1114.069	96.989
700	50.006	125.43	75.42	108.88	-1271.622	-1087.697	81.165
723	51.877	130.48	78.61	110.83	-1271.081	-1082.695	78.240
723	82.317	160.92	78.61	127.61	-1249.073	-1082.695	78.240
800	87.200	173.00	85.80	127.61	-1246.430	-1064.070	69.477
900	92.294	188.69	96.40	127.61	-1242.998	-1041.492	60.447
1000	96.257	202.59	106.33	127.61	-1239.930	-1019.266	53.242
1100	99.381	215.05	115.67	127.61	-1237.209	-997.358	47.361
1200	101.870	226.31	124.44	127.61	-1234.815	-975.680	42.470
1300	103.905	236.56	132.66	127.61	-1232.681	-954.143	38.338
1400	105.616	246.06	140.44	127.61	-1230.752	-932.828	34.804
1500	107.093	254.84	147.75	127.61	-1228.986	-911.562	31.743
1600	108.386	263.09	154.70	127.61	-1227.369	-890.459	29.071
1700	109.529	270.83	161.30	127.61	-1225.899	-869.430	26.715
1800	110.525	278.15	167.62	127.61	-1224.623	-848.466	24.625

MELTING POINT	723	K	BOILING POINT	K
ENTHALPY OF MELTING	22.008	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	9.301	kJ	MOLAR VOLUME	2.7220 J/bar 27.220 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

BOROQ..... M. P. BETA 2300 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.7845 \times 10^2 - 1.0123 \times 10^{-2} T - 4.5398 \times 10^{-5} T^2 + 4.4598 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 723 K)

REFERENCE	247	35	35	COMPILED
		262		6- 2-76

BARIUM OXIDE FORMULA WEIGHT 153.339

BaO: Crystals 298.15 to melting point 2286 K.

TEMP.					FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	72.07	72.07	47.28	-548.100	-520.394	91.171
UNCERTAINTY		0.38	0.38		2.090	2.100	0.368
400	12.400	86.37	73.97	49.98	-547.723	-511.001	66.730
500	20.114	97.73	77.62	51.78	-547.974	-501.805	52.423
600	25.510	107.30	81.79	53.17	-548.930	-492.475	42.874
700	29.546	115.58	86.03	54.33	-548.997	-483.070	36.047
800	32.710	122.91	90.20	55.36	-549.503	-473.613	30.924
900	35.278	129.48	94.20	56.28	-549.525	-464.114	26.937
1000	37.422	135.45	98.03	57.15	-549.489	-454.626	23.747
1100	39.253	140.94	101.69	57.96	-557.762	-444.327	21.099
1200	40.843	146.02	105.18	58.73	-557.845	-434.017	18.892
1300	42.248	150.75	108.50	59.47	-557.768	-423.694	17.024
1400	43.507	155.18	111.67	60.19	-557.580	-413.407	15.424
1500	44.641	159.36	114.72	60.89	-557.241	-403.102	14.037
1600	45.677	163.31	117.63	61.58	-556.830	-392.843	12.825
1700	46.632	167.06	120.43	62.24	-556.347	-382.606	11.756
1800	47.518	170.64	123.12	62.90	-555.812	-372.401	10.807

MELTING POINT	2286	K	BOILING POINT	K
ENTHALPY OF MELTING	58.600	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	9.983	kJ	MOLAR VOLUME	2.5590 J/bar 25.590 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

BARIUM..... ALPHA-BETA 582, BETA-GAMMA 768, H. P. GAMMA 1002,  
B. P. 2169 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 57.218 + 5.3703 \times 10^{-3} T - 1.6681 \times 10^{-5} T^2 + 1.6694 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	33	33	33	COMPILED
	155		58	5-18-76

BROHELITE

FORMULA WEIGHT 25.012

BeO: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		Log K <sub>f</sub>
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	
298.15	0.000	13.77	13.77	25.74	-609.400	-580.078	101.628
UNCERTAINTY		0.04	0.04		2.500	2.500	0.438
400	7.700	22.59	14.89	33.99	-609.693	-570.003	74.435
500	13.478	30.74	17.26	38.89	-609.658	-560.083	58.512
600	18.005	38.14	20.14	42.21	-609.444	-550.179	47.898
700	21.646	44.84	23.19	44.65	-609.121	-540.332	40.320
800	24.645	50.93	26.28	46.55	-608.729	-530.525	34.640
900	27.167	56.50	29.33	48.07	-608.294	-520.769	30.225
1000	29.322	61.64	32.34	49.34	-607.836	-511.076	26.696
1100	31.192	66.39	35.20	50.41	-607.371	-501.419	23.811
1200	32.832	70.82	37.99	51.33	-606.912	-491.814	21.408
1300	34.288	74.96	40.67	52.14	-606.471	-482.243	19.377
1400	35.586	78.85	43.26	52.86	-606.066	-472.702	17.637
1500	36.761	82.52	45.76	53.49	-605.694	-463.194	16.130
1600	37.826	85.99	48.16	54.07	-620.042	-453.266	14.798
1700	38.797	89.28	50.48	54.59	-619.404	-442.851	13.607
1800	39.688	92.42	52.73	55.07	-618.727	-432.499	12.551

MELTING POINT	2681	K	BOILING POINT	K
ENTHALPY OF MELTING	65.610	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	2.883	kJ	MOLAR VOLUME	0.8309 J/bar 8.309 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

BERYLLIUM.. ALPHA-BETA 1527, M. P. 1560 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 69.936 + 1.8288 \times 10^{-4} T - 6.3574 \times 10^{-8} T^{0.5} - 6.7671 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	32	215	215	COMPILED
	261			6- 8-76

## BERYLLIUM OXIDE (BETA)

FORMULA WEIGHT 25.012

BeO: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	16.54	16.54	25.56	-601.785	-573.289	100.438
UNCERTAINTY		0.03	0.03		3.500	3.500	0.613
400	7.650	25.32	17.67	33.84	-602.098	-563.500	73.586
500	13.432	33.45	20.02	38.85	-602.066	-553.846	57.860
600	17.968	40.85	22.88	42.26	-601.851	-544.212	47.378
700	21.626	47.56	25.93	44.75	-601.520	-534.635	39.895
800	24.639	53.67	29.03	46.64	-601.119	-525.107	34.286
900	27.167	59.25	32.08	48.13	-600.679	-515.629	29.926
1000	29.328	64.38	35.05	49.35	-600.215	-506.195	26.441
1100	31.196	69.14	37.94	50.38	-599.751	-496.824	23.592
1200	32.833	73.56	40.73	51.27	-599.296	-487.486	21.220
1300	34.282	77.70	43.42	52.06	-598.863	-478.197	19.214
1400	35.579	81.58	46.00	52.79	-598.461	-468.919	17.496
1500	36.749	85.25	48.50	53.47	-598.097	-459.692	16.008
1600	37.815	88.72	50.91	54.12	-612.444	-450.036	14.692
1700	38.793	92.02	53.23	54.76	-611.796	-439.901	13.517
1800	39.698	95.17	55.47	55.39	-611.094	-429.816	12.473

MELTING POINT	2720	K	BOILING POINT		K
ENTHALPY OF MELTING	59.120	kJ	ENTHALPY OF VAPORIZATION		kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME		J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

BERYLLIUM.. ALPHA-BETA 1527, M. P. 1560 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 89.212 - 1.1200 \times 10^{-2} T + 3.0413 \times 10^{-6} T^2 - 9.9399 \times 10^2 T^{-0.5} - 2.6822 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	32	32	32	COMPILED	7-29-76
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BISMITE

FORMULA WEIGHT 465.959

Bi<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to melting point 1098 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	151.46	151.46	113.51	-573.877	-493.453	86.451
UNCERTAINTY		2.09	2.09		1.255	1.464	0.256
400	29.325	185.29	155.96	116.90	-571.969	-466.275	60.890
500	47.184	211.74	164.56	120.24	-570.217	-440.062	45.973
600	59.638	233.96	174.32	123.58	-591.288	-411.873	35.857
700	69.011	253.26	184.25	126.91	-589.459	-382.105	28.513
800	76.457	270.42	193.96	130.25	-587.257	-352.637	23.025

MELTING POINT	1098	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	4.9730 J/bar 49.730 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

BISMUTH.... M. P. 544.5, B. P. 1835 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.0356 \times 10^2 + 3.3360 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 800 K)

REFERENCE	115	262	262	COMPILED
			161	5-26-76

## CARBON MONOXIDE

FORMULA WEIGHT 28.010

CO: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	197.67	197.67	29.14	-110.530	-137.171	24.032
UNCERTAINTY		0.03	0.03		0.170	0.170	0.030
400	7.375	206.19	198.81	29.10	-110.136	-146.346	19.111
500	11.792	212.75	200.96	29.79	-110.059	-155.409	16.236
600	14.857	218.26	203.40	30.58	-110.206	-164.473	14.319
700	17.159	223.03	205.87	31.34	-110.509	-173.496	12.946
800	18.975	227.26	208.28	32.03	-110.925	-182.465	11.914
900	20.456	231.07	210.61	32.64	-111.429	-191.385	11.108
1000	21.705	234.53	212.82	33.18	-111.984	-200.224	10.459
1100	22.771	237.72	214.95	33.67	-112.587	-209.024	9.926
1200	23.697	240.67	216.97	34.10	-113.221	-217.771	9.479
1300	24.513	243.41	218.90	34.49	-113.877	-226.444	9.099
1400	25.236	245.98	220.74	34.85	-114.553	-235.079	8.771
1500	25.891	248.40	222.51	35.17	-115.230	-243.675	8.486
1600	26.480	250.68	224.20	35.47	-115.917	-252.213	8.234
1700	27.016	252.84	225.82	35.74	-116.609	-260.726	8.011
1800	27.508	254.89	227.38	35.99	-117.303	-269.169	7.811

MELTING POINT	68.05 K	BOILING POINT	81.61 K
ENTHALPY OF MELTING	0.837 kJ	ENTHALPY OF VAPORIZATION	6.042 kJ
$H_{298}^0 - H_0^0$	8.673 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_P^0 = 45.730 - 9.7115 \times 10^{-5} T - 4.1469 \times 10^{-2} T^{-0.5} + 6.6270 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	35	35	COMPILED 5-24-76
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CARBON DIOXIDE FORMULA WEIGHT 44.010

CO<sub>2</sub>: Ideal gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	213.79	213.79	37.13	-393.510	-394.375	69.093
UNCERTAINTY		0.04	0.04		0.130	0.167	0.029
400	9.975	225.28	215.31	41.23	-393.588	-394.660	51.538
500	16.588	234.87	218.28	44.65	-393.685	-394.920	41.257
600	21.505	243.26	221.75	47.42	-393.823	-395.149	34.401
700	25.371	250.74	225.37	49.66	-393.994	-395.359	29.502
800	28.526	257.50	228.97	51.49	-394.184	-395.544	25.826
900	31.167	263.65	232.48	53.02	-394.388	-395.694	22.966
1000	33.416	269.31	235.89	54.30	-394.600	-395.830	20.676
1100	35.365	274.53	239.17	55.38	-394.814	-395.936	18.802
1200	37.072	279.39	242.32	56.30	-395.027	-396.035	17.239
1300	38.582	283.93	245.35	57.10	-395.236	-396.107	15.916
1400	39.929	288.19	248.26	57.78	-395.442	-396.171	14.781
1500	41.140	292.20	251.06	58.38	-395.640	-396.225	13.798
1600	42.234	295.98	253.75	58.89	-395.834	-396.250	12.936
1700	43.228	299.57	256.34	59.34	-396.023	-396.293	12.177
1800	44.134	302.97	258.84	59.74	-396.211	-396.282	11.500

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	9.364 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 87.820 - 2.6442 \times 10^{-3} T - 9.9886 \times 10^2 T^{-0.5} + 7.0641 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	35	35	COMPILED
		96		5-24-76

CALCIUM OXIDE FORMULA WEIGHT 56.079

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CaO: Crystals 298.15 to 1800K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	38.21	38.21	42.12	-635.089	-603.487	105.729
UNCERTAINTY		0.13	0.13		0.879	0.900	0.158
400	11.375	51.31	39.93	46.65	-634.672	-592.746	77.405
500	18.684	61.99	43.31	48.98	-634.105	-582.330	60.836
600	23.863	71.06	47.20	50.46	-633.569	-572.024	49.799
700	27.743	78.92	51.18	51.53	-633.161	-561.803	41.922
800	30.771	85.86	55.09	52.39	-633.672	-551.540	36.012
900	33.211	92.07	58.86	53.10	-633.570	-541.275	31.415
1000	35.235	97.70	62.47	53.73	-633.837	-531.007	27.737
1100	36.943	102.85	65.91	54.30	-634.485	-520.701	24.726
1200	38.412	107.60	69.19	54.84	-642.458	-509.696	22.187
1300	39.695	112.01	72.31	55.34	-641.671	-498.671	20.037
1400	40.829	116.12	75.29	55.82	-640.855	-487.695	18.196
1500	41.845	119.99	78.15	56.28	-640.001	-476.786	16.603
1600	42.761	123.64	80.88	56.73	-639.117	-465.941	15.211
1700	43.596	127.09	83.49	57.17	-638.201	-455.137	13.985
1800	44.362	130.37	86.01	57.60	-790.750	-441.040	12.799

MELTING POINT	3200 K	BOILING POINT	K
ENTHALPY OF MELTING	79.496 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	6.749 kJ	MOLAR VOLUME	1.6764 J/bar 16.764 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 52.422 + 3.6734 \times 10^{-3} T - 50.988 T^{-0.5} - 7.5068 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

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REFERENCE	33	33	33	COMPILED 5-18-76
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PORTLANDITE

FORMULA WEIGHT 74.095

Ca(OH)<sub>2</sub>: Crystals 298.15 to 700 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	83.39	83.39	87.49	-986.085	-898.408	157.398
UNCERTAINTY		0.42	0.42		1.255	1.300	0.228
400	23.725	110.69	86.96	97.92	-985.203	-868.474	113.412
500	39.234	133.27	94.04	104.17	-983.757	-839.483	87.701
600	50.418	152.64	102.22	108.21	-982.072	-810.791	70.586
700	58.877	169.54	110.66	110.87	-980.365	-782.407	58.384

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	14.159 kJ	MOLAR VOLUME	3.3056 J/bar 33.056 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, H. P. BETA 1112, B. P. 1755 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.8667 \times 10^2 - 2.1911 \times 10^{-2} T - 1.5998 \times 10^3 T^{-0.5}$$

(EQUATION VALID FROM 298 - 700 K)

REFERENCE	32	32	32	COMPILED
		86	86	7- 1-76

## CERIANITE

FORMULA WEIGHT 172.119

CeO<sub>2</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	62.30	62.30	61.63	-1088.680	-1025.380	179.643
UNCERTAINTY		0.08	0.08		1.464	2.929	0.513
400	16.525	81.33	64.80	67.52	-1087.906	-1003.866	131.092
500	27.080	96.78	69.70	70.84	-1086.939	-982.964	102.690
600	34.573	109.91	75.34	73.12	-1085.943	-962.265	83.773
700	40.209	121.31	81.10	74.86	-1084.994	-941.725	70.273
800	44.631	131.41	86.78	76.29	-1084.125	-921.325	60.157
900	48.222	140.47	92.25	77.52	-1083.352	-901.012	52.294
1000	51.206	148.69	97.48	78.62	-1085.687	-880.787	46.008
1100	53.745	156.23	102.49	79.63	-1090.501	-860.172	40.846
1200	55.942	163.20	107.26	80.57	-1089.810	-839.262	36.532
1300	57.870	169.69	111.82	81.45	-1089.066	-818.432	32.885
1400	59.586	175.75	116.16	82.29	-1088.267	-797.627	29.760
1500	61.125	181.46	120.33	83.10	-1087.419	-776.904	27.054
1600	62.523	186.85	124.33	83.88	-1086.517	-756.245	24.689
1700	63.802	191.95	128.15	84.64	-1085.561	-735.616	22.603
1800	64.980	196.81	131.83	85.38	-1084.551	-715.065	20.751

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	10.368 kJ	MOLAR VOLUME	2.3853 J/bar 23.853 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CERIUM..... BETA-GAMMA 999, M. P. 1071 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 80.292 + 5.6994 \times 10^{-3} T - 2.0990 \times 10^{-6} T^2 + 7.2941 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	130	279	235	COMPILED
			8	6- 2-76

CERIUM SESQUIOXIDE (HEXAGONAL,  $\alpha$ )

FORMULA WEIGHT 328.238

Ce<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	150.62	150.62	124.37	-1796.200	-1707.940	299.225
UNCERTAINTY		4.18	4.18		8.400	8.400	1.472
400	31.425	186.82	155.39	128.13	-1793.790	-1678.148	219.145
500	51.400	216.09	164.69	134.00	-1791.054	-1649.544	172.327
600	65.525	240.90	175.38	138.11	-1788.273	-1621.506	141.165
700	76.136	262.45	186.31	141.40	-1785.571	-1593.932	118.941
800	84.475	281.52	197.05	144.25	-1783.000	-1566.732	102.298
900	91.267	298.66	207.39	146.84	-1780.585	-1539.826	89.370
1000	96.942	314.25	217.31	149.27	-1784.337	-1513.197	79.042

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	21.464 kJ	MOLAR VOLUME	4.7750 J/bar 47.750 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CERIUM..... BETA-GAMMA 999, M. P. 1071 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.3066 \times 10^2 + 2.0315 \times 10^{-2} T - 1.7053 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	202	113	235	COMPILED
			105	5-18-76

CERIUM SESQUIOXIDE (HEXAGONAL,  $\beta$ )

FORMULA WEIGHT 328.238

Ce<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1500 K.

TEMP.					FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$	$\frac{S_T^0 - S_{298}^0}{T}$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	0.00	---	131.01	---	---	---
UNCERTAINTY							
400	33.350	38.45	---	134.21	---	---	---
500	54.036	68.94	---	139.15	---	---	---
600	68.578	94.69	---	143.35	---	---	---
700	79.539	117.08	---	147.21	---	---	---
800	88.227	136.98	---	150.88	---	---	---
900	95.389	154.96	---	154.45	---	---	---
1000	101.469	171.41	---	157.95	---	---	---
1100	106.761	186.63	---	161.41	---	---	---
1200	111.458	200.82	---	164.84	---	---	---
1300	115.695	214.15	---	168.24	---	---	---
1400	119.571	226.74	---	171.63	---	---	---
1500	123.153	238.70	---	175.02	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CERIUM..... BETA-GAMMA 999, M. P. 1071 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.2532 \times 10^2 + 3.3341 \times 10^{-2} T - 7.1123 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE 202

COMPILED  
6- 8-76

COBALTOUS OXIDE FORMULA WEIGHT 74.933

CoO: Crystals 298.15 to melting point 2078 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	52.97	52.97	43.32	-237.940	-214.194	37.526
UNCERTAINTY		0.34	0.34		1.255	1.297	0.227
400	13.525	67.18	53.65	51.86	-236.659	-205.725	26.865
500	21.456	79.03	57.57	53.99	-235.611	-198.111	20.697
600	26.930	88.93	62.00	54.50	-234.659	-190.700	16.602
700	30.880	97.34	66.46	54.66	-233.867	-183.439	13.688
800	33.865	104.66	70.80	54.89	-233.667	-176.223	11.506
900	36.222	111.14	74.92	55.29	-233.214	-169.062	9.812
1000	38.158	117.00	78.84	55.91	-232.949	-161.959	8.460
1100	39.807	122.36	82.55	56.74	-232.896	-154.862	7.354
1200	41.259	127.34	86.08	57.75	-233.105	-147.755	6.432
1300	42.572	132.01	89.44	58.94	-233.644	-140.629	5.651
1400	43.786	136.43	92.64	60.28	-234.606	-133.456	4.979
1500	44.936	140.63	95.69	61.75	-236.075	-126.155	4.393
1600	46.035	144.67	98.63	63.33	-238.172	-118.772	3.878
1700	47.102	148.56	101.46	65.02	-241.004	-111.235	3.418
1800	48.146	152.32	104.17	66.80	-248.550	-104.424	3.030

MELTING POINT	2078	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	1.1640 J/bar 11.640 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

COBALT..... ALPHA-BETA 700, CURIE P. 1394, M. P. BETA 1768 K.

HEAT CAPACITY EQUATION

$$C_P^0 = - 30.468 + 2.9459 \times 10^{-2} T + 1.9317 \times 10^{-5} T^2 - 4.1658 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	129	120	263	COMPILED 6-8-76
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## ESKOLAITE

FORMULA WEIGHT 151.990

Cr<sub>2</sub>O<sub>3</sub>: Beta crystals 298.15 to melting point 2603 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	81.17	81.17	101.34	-1134.700	-1053.056	184.492
UNCERTAINTY		1.25	1.25		8.370	8.400	1.472
400	28.125	113.45	85.32	113.64	-1132.992	-1025.370	133.900
500	45.686	139.30	93.61	117.85	-1131.195	-998.680	104.332
600	57.953	161.05	103.10	120.57	-1129.398	-972.345	84.650
700	67.049	179.79	112.74	122.60	-1127.690	-946.299	70.614
800	74.097	196.27	122.17	124.24	-1126.126	-920.506	60.103
900	79.756	210.99	131.23	125.67	-1124.741	-894.863	51.937
1000	84.408	224.30	139.89	126.97	-1123.581	-869.391	45.413
1100	88.332	236.45	148.12	128.17	-1122.661	-844.020	40.079
1200	91.700	247.66	155.96	129.32	-1122.011	-818.729	35.639
1300	94.635	258.05	163.41	130.42	-1121.647	-793.464	31.882
1400	97.229	267.76	170.53	131.49	-1121.597	-768.239	28.663
1500	99.549	276.86	177.31	132.54	-1121.869	-742.968	25.873
1600	101.642	285.45	183.81	133.57	-1122.491	-717.717	23.431
1700	103.550	293.58	190.03	134.58	-1123.476	-692.397	21.275
1800	105.302	301.30	196.00	135.59	-1124.843	-667.012	19.356

MELTING POINT	2603	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.9090 J/bar 29.090 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CHROMIUM... M. P. 2130 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.1902 \times 10^2 + 9.4964 \times 10^{-3} T - 3.4045 T^{-0.5} - 1.4419 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	33	33	33	COMPILED
			158	6- 8-76



CESIUM HYDROXIDE

FORMULA WEIGHT 149.913

CSOH: Crystals 298.15 to 1000 K. CsOH melts at 588 K. The heat capacities over the range 298.15 to 1000 K have been estimated.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	98.74	98.74	67.86	-416.726	-370.690	64.944
UNCERTAINTY		4.18	4.18		0.837	0.850	0.149
400	18.127	119.61	101.49	74.39	-418.538	-354.292	46.266
500	44.936	152.58	107.64	82.42	-409.618	-338.759	35.390
600	51.352	167.78	116.43	81.59	-407.182	-324.805	28.277
700	55.970	180.68	124.71	81.59	-404.549	-311.288	23.229
800	59.434	191.85	132.42	81.59	-401.965	-298.137	19.466
900	62.128	201.71	139.59	81.59	-399.639	-285.297	16.558
1000	64.282	210.53	146.25	81.59	-463.737	-268.617	14.031

MELTING POINT	588	K	BOILING POINT	K
ENTHALPY OF MELTING	4.561	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	J/bar

TRANSITIONS IN REFERENCE STATE ELEMENTS

CESIUM..... M. P. 301.55, B. P. 942 K.

REFERENCE	32	32	32	COMPILED
				10-11-74

TENORITE

FORMULA WEIGHT 79.545

CuO: Crystals 298.15 to 1400 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	42.63	42.63	42.30	-157.320	-129.564	22.699
UNCERTAINTY		0.21	0.21		1.255	1.297	0.227
400	11.475	55.83	44.36	47.07	-156.785	-120.151	15.690
500	18.832	66.60	47.77	49.32	-156.071	-111.076	11.604
600	24.043	75.73	51.69	50.79	-155.289	-102.150	8.893
700	27.951	83.65	55.70	51.98	-154.477	-93.360	6.967
800	31.021	90.66	59.64	53.05	-153.640	-84.684	5.529
900	33.522	96.97	63.45	54.09	-152.780	-76.118	4.418
1000	35.635	102.72	67.09	55.13	-151.877	-67.647	3.534
1100	37.455	108.02	70.56	56.18	-150.936	-59.262	2.814
1200	39.059	112.96	73.90	57.24	-149.951	-50.981	2.219
1300	40.500	117.58	77.08	58.33	-148.912	-42.767	1.718
1400	41.814	121.94	80.13	59.43	-146.107	-34.355	1.282

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	7.100 kJ	MOLAR VOLUME	1.2220 J/bar 12.220 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

COPPER..... M. P. 1357 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 30.967 + 1.3742 \times 10^{-2} T + 3.6926 \times 10^{-5} T^{0.5} - 1.2578 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	164	120	263	COMPILED
			164	5-28-76

CUPRITE

FORMULA WEIGHT 143.091

Cu<sub>2</sub>O: Crystals 298.15 to melting point 1509 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	93.14	93.14	62.59	-168.610	-146.030	25.584
UNCERTAINTY		1.67	1.67		6.276	6.318	1.107
400	16.475	112.13	95.65	67.23	-168.618	-138.312	18.062
500	27.088	127.62	100.53	71.54	-168.356	-130.751	13.660
600	34.748	140.93	106.18	74.32	-167.925	-123.270	10.732
700	40.536	152.53	111.99	76.06	-167.428	-115.873	8.647
800	45.060	162.77	117.71	77.35	-166.917	-108.538	7.087
900	48.722	171.96	123.24	78.67	-166.401	-101.268	5.877
1000	51.796	180.33	128.53	80.41	-165.851	-94.071	4.914
1100	54.502	188.10	133.60	82.84	-165.192	-86.916	4.127
1200	56.996	195.45	138.45	86.18	-164.344	-79.845	3.476
1300	59.404	202.51	143.11	90.59	-163.201	-72.839	2.927
1400	61.821	209.42	147.60	96.21	-188.235	-65.380	2.439
1500	64.341	216.29	151.95	103.13	-186.375	-56.631	1.972

MELTING POINT	1509	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.3437 J/bar 23.437 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

COPPER..... M. P. 1357 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 4.2602 \times 10^{-2} - 0.25076 T + 9.2444 \times 10^{-5} T^2 - 6.0778 \times 10^{-8} T^{-0.5} + 4.8982 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	164	263	263 164	COMPILED 6-15-76
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## DYSPROSIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 372.998

Dy<sub>2</sub>O<sub>3</sub>: Alpha crystals 298.15 to 1590 K. Beta crystals 1590 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	149.79	149.79	111.74	-1863.130	-1771.385	310.341
UNCERTAINTY		0.85	0.85		3.930	4.000	0.701
400	30.275	184.64	154.36	123.67	-1861.284	-1740.298	227.261
500	49.402	212.72	163.32	127.59	-1858.919	-1710.314	178.676
600	62.595	236.16	173.56	129.36	-1856.459	-1680.836	140.330
700	72.219	256.19	183.97	130.53	-1854.051	-1651.758	123.256
800	79.576	273.69	194.11	131.64	-1851.763	-1623.007	105.972
900	85.422	289.27	203.85	132.87	-1849.641	-1594.545	92.545
1000	90.240	303.34	213.10	134.28	-1847.705	-1566.315	81.816
1100	94.315	316.21	221.90	135.87	-1846.014	-1538.245	73.045
1200	97.851	328.10	230.25	137.65	-1844.606	-1510.316	65.743
1300	100.985	339.20	238.21	139.58	-1843.528	-1482.518	59.569
1400	103.814	349.62	245.81	141.66	-1842.843	-1454.791	54.279
1500	106.412	359.47	253.06	143.88	-1842.596	-1427.081	49.696
1590	108.592	367.91	259.32	145.97	-1842.373	-1402.142	46.064
1590	109.051	368.37	259.32	144.23	-1841.644	-1402.142	46.064
1600	109.271	369.28	260.01	144.23	-1842.141	-1399.397	45.332
1700	111.328	378.03	266.70	144.23	-1872.523	-1371.321	41.782
1800	113.156	386.27	273.11	144.23	-1873.665	-1341.693	38.581

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	21.087 kJ	MOLAR VOLUME	4.5683 J/bar 45.683 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

DYSPROSIUM. ALPHA-BETA 1657, M. P. 1682 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 38.243 + 3.7210 \times 10^{-2} T + 2.0124 \times 10^{-3} T^{0.5} - 4.8131 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1590 K)

REFERENCE	202	235	235	103	COMPILED
					5-18-76

ERBIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 382.518

Er<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol
298.15	0.000	155.64	155.64	118.09	-1897.860	-1808.879	316.909
UNCERTAINTY		0.85	0.85		1.920	2.000	0.350
400	28.250	190.36	162.11	118.77	-1896.848	-1779.486	232.378
500	46.564	217.09	170.53	120.96	-1895.178	-1750.348	182.858
600	59.158	239.35	180.19	123.28	-1893.505	-1721.536	149.874
700	68.476	258.52	190.04	125.43	-1891.841	-1693.013	126.335
800	75.716	275.39	199.67	127.35	-1890.211	-1664.703	108.694
900	81.544	290.49	208.95	129.04	-1888.649	-1636.613	94.987
1000	86.376	304.17	217.79	130.55	-1887.171	-1608.691	84.030
1100	90.455	316.68	226.23	131.89	-1885.822	-1580.902	75.071
1200	93.958	328.21	234.25	133.09	-1884.627	-1553.253	67.612
1300	97.012	338.90	241.89	134.18	-1883.606	-1525.664	61.302
1400	99.700	348.88	249.18	135.16	-1882.797	-1498.161	55.897
1500	102.096	358.24	256.14	136.05	-1882.214	-1470.734	51.216
1600	104.244	367.05	262.81	136.87	-1881.888	-1443.320	47.120
1700	106.186	375.37	269.18	137.63	-1881.844	-1415.900	43.505
1800	107.953	383.25	275.30	138.32	-1921.861	-1388.377	40.290

MELTING POINT

K

BOILING POINT

K

ENTHALPY OF MELTING

kJ

ENTHALPY OF VAPORIZATION

kJ

$H_{298}^0 - H_0^0$

20.000 kJ

MOLAR VOLUME

4.4171 J/bar  
44.171 cm<sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ERBIUM..... M. P. 1795 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.6353 \times 10^2 + 6.9435 \times 10^{-5} T - 1.0957 \times 10^{-8} T^{0.5} + 1.5992 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 207

235

235

COMPILED  
5-19-76

## EUROPIUM OXIDE

FORMULA WEIGHT 167.959

EuO: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		Log K <sub>f</sub>
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	62.76	62.76	48.74	-592.040	-556.082	97.424
UNCERTAINTY		0.85	0.85		8.370	8.370	1.466
400	12.525	77.21	64.68	49.64	-591.338	-543.908	71.027
500	20.030	88.37	68.34	50.42	-590.736	-532.121	55.591
600	25.157	97.63	72.47	51.16	-590.246	-520.439	45.308
700	28.921	105.57	76.65	51.87	-589.808	-508.846	37.971
800	31.835	112.55	80.72	52.58	-589.468	-497.304	32.471
900	34.178	118.78	84.60	53.29	-589.285	-485.794	28.195
1000	36.126	124.43	88.30	53.99	-589.309	-474.299	24.775
1100	37.781	129.61	91.83	54.68	-598.764	-462.705	21.972
1200	39.218	134.40	95.18	55.38	-598.848	-450.330	19.602
1300	40.488	138.86	98.37	56.07	-598.880	-437.953	17.597
1400	41.629	143.04	101.41	56.77	-598.857	-425.565	15.878
1500	42.659	146.98	104.32	57.46	-598.786	-413.191	14.389
1600	43.605	150.71	107.10	58.15	-598.656	-400.824	13.086
1700	44.481	154.25	109.77	58.84	-598.467	-388.458	11.936
1800	45.298	157.64	112.34	59.53	-598.221	-376.119	10.915

MELTING POINT	2247	K	BOILING POINT		K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION		kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.0475	J/bar
				20.475	cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

EUROPIUM... M. P. 1090, B. P. 1868 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 47.124 + 6.9013 \times 10^{-3} T - 3.9277 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	166	235	235	COMPILED
				5-19-76

EUROPIUM SESQUIOXIDE (MONOCLINIC)

FORMULA WEIGHT 351.918

Eu<sub>2</sub>O<sub>3</sub>: Alpha crystals 298.15 to 895 K. Beta crystals 895 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	146.44	146.44	115.69	-1651.420	-1555.158	272.458
UNCERTAINTY		8.50	8.50		8.400	8.400	1.472
400	31.500	182.68	151.18	129.62	-1648.948	-1522.618	198.834
500	51.810	212.36	160.55	135.88	-1645.981	-1491.386	155.805
600	66.132	237.46	171.33	139.28	-1642.967	-1460.732	127.169
700	76.740	259.10	182.36	141.34	-1639.982	-1430.612	106.754
800	84.902	278.06	193.16	142.67	-1637.210	-1400.878	91.468
895	90.967	294.00	203.03	143.93	-1635.043	-1372.924	80.128
895	91.685	294.72	203.03	146.33	-1634.400	-1372.924	80.128
900	91.956	295.49	203.53	146.41	-1634.289	-1371.471	79.598
1000	97.482	311.00	213.52	147.98	-1632.075	-1342.405	70.120
1100	102.144	325.18	223.04	149.56	-1648.728	-1313.360	62.367
1200	106.161	338.26	232.10	151.13	-1646.642	-1282.952	55.846
1300	109.681	350.42	240.74	152.71	-1644.454	-1252.738	50.336
1400	112.807	361.79	248.98	154.28	-1642.163	-1222.681	45.619
1500	115.627	372.49	256.86	155.86	-1639.751	-1192.796	41.537
1600	118.191	382.60	264.41	157.43	-1637.226	-1163.090	37.971
1700	120.545	392.19	271.64	159.01	-1634.576	-1133.544	34.830
1800	122.726	401.32	278.59	160.58	-1631.803	-1104.133	32.041

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	4.4020 J/bar 44.020 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

EUROPIUM... M. P. 1090, B. P. 1868 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.4702 \times 10^{-2} - 2.7846 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 895 K)

$$C_P^0 = 1.3223 \times 10^{-2} + 1.5752 \times 10^{-2} T$$

(EQUATION VALID FROM 895 - 1800 K)

REFERENCE	210	281	235	COMPILED
			57	5-18-76

EUROPIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 351.918

Eu<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$\frac{S_T^0}{S_{298}^0} -$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $f$
298.15	0.000	0.00	---	120.49	---	---	---
UNCERTAINTY							
400	33.000	37.13	---	131.40	---	---	---
500	53.302	67.13	---	137.18	---	---	---
600	67.622	92.50	---	141.05	---	---	---
700	78.330	114.47	---	144.01	---	---	---
800	86.700	133.87	---	146.49	---	---	---
900	93.467	151.25	---	148.70	---	---	---
1000	99.094	167.03	---	150.73	---	---	---
1100	103.876	181.48	---	152.64	---	---	---
1200	108.017	194.85	---	154.48	---	---	---
1300	111.661	207.28	---	156.27	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.8290 J/bar 48.290 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

EUROPIUM... M. P. 1090, B. P. 1868 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.3665 \times 10^2 + 1.5936 \times 10^{-2} T - 1.8595 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1350 K)

REFERENCE 210

COMPILED  
5-18-76



WUSTITE

FORMULA WEIGHT 68.887

Fe<sub>0.947</sub>O: Crystals 298.15 to melting point 1652 K. Liquid 1652 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	57.59	57.59	48.12	-266.270	-245.155	42.950
UNCERTAINTY		0.42	0.42		0.837	0.879	0.154
400	12.875	72.41	59.53	51.98	-265.148	-238.104	31.093
500	20.790	84.12	63.33	52.78	-264.109	-231.460	24.181
600	26.143	93.77	67.63	53.04	-263.293	-225.011	19.589
700	30.007	101.97	71.96	53.38	-262.732	-218.700	16.320
800	32.961	109.13	76.17	53.94	-262.481	-212.430	13.870
900	35.333	115.53	80.20	54.75	-262.632	-206.144	11.964
1000	37.327	121.35	84.02	55.80	-263.430	-199.832	10.438
1100	39.062	126.72	87.66	57.05	-265.009	-193.367	9.182
1200	40.618	131.74	91.12	58.47	-265.646	-186.860	8.134
1300	42.052	136.49	94.44	60.05	-264.764	-180.373	7.247
1400	43.400	141.00	97.60	61.76	-263.809	-173.925	6.489
1500	44.681	145.32	100.64	63.58	-262.742	-167.522	5.834
1600	45.921	149.48	103.56	65.50	-261.574	-161.216	5.263
1652	46.204	151.35	105.14	66.54	-261.521	-158.097	4.999
1652	65.174	170.32	105.14	67.90	-230.182	-158.097	4.999
1700	65.251	172.18	106.93	67.90	-230.607	-155.879	4.790
1800	65.398	176.06	110.66	67.90	-229.600	-151.478	4.396

MELTING POINT	1652 K	BOILING POINT	K
ENTHALPY OF MELTING	31.338 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	9.464 kJ	MOLAR VOLUME	1.2040 J/bar 12.040 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

HEAT CAPACITY EQUATION

$$C_P^0 = - 19.296 + 3.0165 \times 10^{-2} T + 1.5009 \times 10^{-5} T^2 - 2.5333 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1652 K)

REFERENCE	44	120	109	COMPILED
		247	247	6-11-76

FERROUS OXIDE (STOICHIOMETRIC) FORMULA WEIGHT 71.846

FeO: Crystals 298.15 to 1652 K. Liquid 1652 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	59.80	59.80	49.92	-272.043	-251.156	44.002
UNCERTAINTY		1.67	1.67		2.092	2.176	0.381
400	12.950	74.72	61.77	51.74	-271.032	-244.171	31.886
500	20.874	86.45	65.58	53.42	-270.131	-237.553	24.817
600	26.425	96.33	69.90	54.90	-269.349	-231.115	20.120
700	30.589	104.89	74.30	56.20	-268.725	-224.813	16.776
800	33.864	112.47	78.61	57.36	-268.352	-218.568	14.271
900	36.533	119.29	82.76	58.40	-268.363	-212.321	12.323
1000	38.768	125.49	86.72	59.36	-269.057	-206.064	10.764
1100	40.680	131.19	90.51	60.24	-270.603	-199.668	9.482
1200	42.345	136.47	94.12	61.06	-271.208	-193.235	8.411
1300	43.815	141.39	97.58	61.84	-270.287	-186.812	7.506
1400	45.129	146.00	100.87	62.57	-269.391	-180.441	6.732
1500	46.315	150.34	104.02	63.27	-268.480	-174.094	6.063
1600	47.396	154.44	107.04	63.95	-267.597	-167.835	5.479
1652	47.922	157.80	109.88	64.29	-267.168	-166.727	5.272
1652	61.351	171.23	109.88	68.20	-244.983	-166.727	5.272
1700	61.544	173.10	111.56	68.20	-245.551	-164.321	5.049
1800	61.914	176.99	115.08	68.20	-244.734	-159.516	4.629

MELTING POINT	1652 K	BOILING POINT	K
ENTHALPY OF MELTING	22.185 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	1.2000 J/bar 12.000 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

#### HEAT CAPACITY EQUATION

$$C_P^0 = 67.352 + 3.7580 \times 10^{-3} T - 3.8167 \times 10^{-6} T^{0.5} + 3.1570 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1652 K)

REFERENCE 247 247 247 COMPILED 5-24-76

HEMATITE

FORMULA WEIGHT 159.692

Fe<sub>2</sub>O<sub>3</sub>: Alpha crystals 298.15 to 950 K. Beta crystals 950 to melting point 1895 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>p</sub> <sup>0</sup> J/mol·K			
298.15	0.000	87.40	87.40	103.85	-824.640	-742.683	130.116
UNCERTAINTY		0.21	0.21		1.255	1.297	0.227
400	28.800	120.50	91.70	120.91	-822.970	-714.899	93.357
500	48.338	148.69	100.35	131.39	-820.565	-688.130	71.889
600	62.833	173.34	110.51	139.01	-817.888	-661.886	57.623
700	74.241	195.33	121.09	146.53	-815.113	-636.156	47.471
800	83.844	215.48	131.64	156.06	-812.285	-610.777	39.880
900	92.556	234.58	142.02	169.20	-809.359	-585.703	33.993
950	96.224	243.81	147.59	177.51	-807.736	-573.749	31.547
950	98.168	245.76	147.59	151.69	-805.888	-573.749	31.547
1000	100.551	252.71	152.16	148.49	-807.000	-560.954	29.301
1100	104.666	266.61	161.94	143.55	-809.223	-536.201	25.462
1200	107.772	278.96	171.19	140.74	-810.146	-511.419	22.262
1300	110.267	290.18	179.91	140.07	-808.368	-486.665	19.555
1400	112.429	300.60	188.17	141.42	-806.775	-462.023	17.238
1500	114.459	310.45	195.99	144.64	-805.076	-437.399	15.232
1600	116.489	319.93	203.44	149.58	-803.176	-412.971	13.482
1700	118.618	329.19	210.57	156.06	-803.249	-388.584	11.940
1800	120.909	338.32	217.41	163.95	-801.129	-364.167	10.568

MELTING POINT	1895 K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	15.560 kJ	MOLAR VOLUME	3.0274 J/bar 30.274 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

HEAT CAPACITY EQUATIONS

$$C_p^0 = - 838.61 + 86.525 T^{0.5} - 2.3434 T + 6.0519 \times 10^{-4} T^2 + 2.7821 \times 10^{-4} T^{-1}$$

(EQUATION VALID FROM 298 - 950 K)

$$C_p^0 = -1.0957 \times 10^3 + 0.27267 T + 3.3960 \times 10^{-4} T^{0.5} - 1.0239 \times 10^8 T^{-2}$$

(EQUATION VALID FROM 950 - 1800 K)

REFERENCE	44	78	84	COMPILED
	78	247		6-11-76

## MAGNETITE

FORMULA WEIGHT 231.539

Fe<sub>3</sub>O<sub>4</sub>: Alpha crystals 298.15 to 848 K. Beta crystals 848 to melting point  
1870 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	146.14	146.14	150.79	-1115.726	-1012.566	177.398
UNCERTAINTY		0.42	0.42		2.092	2.134	0.374
400	41.825	194.24	152.41	176.03	-1113.015	-977.691	127.674
500	70.428	235.41	164.98	192.45	-1109.131	-944.253	98.646
600	92.007	271.81	179.80	207.63	-1104.631	-911.679	79.369
700	109.994	305.36	195.37	229.74	-1099.267	-879.995	65.666
800	127.047	338.21	211.16	265.64	-1092.209	-849.125	55.442
848	134.099	353.81	219.71	289.43	-1088.391	-835.281	51.451
848	136.949	356.66	219.71	219.99	-1085.646	-835.281	51.451
900	141.144	368.15	227.01	213.93	-1085.915	-819.068	47.538
1000	147.986	390.24	242.25	205.97	-1086.433	-789.434	41.236
1100	153.031	409.63	256.60	201.45	-1090.416	-759.472	36.064
1200	156.962	427.06	270.10	199.28	-1092.184	-729.441	31.752
1300	160.188	442.98	282.79	198.76	-1089.761	-699.415	28.103
1400	162.964	457.72	294.76	199.43	-1087.639	-669.504	24.980
1500	165.440	471.53	306.09	200.99	-1085.600	-639.647	22.275
1600	167.729	484.57	316.84	203.23	-1083.668	-610.018	19.915
1700	169.896	496.97	327.07	205.99	-1085.295	-580.354	17.832
1800	171.988	508.84	336.85	209.15	-1084.411	-550.587	15.978

MELTING POINT	1870	K	BOILING POINT	K
ENTHALPY OF MELTING	138.072	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	24.573	kJ	MOLAR VOLUME	4.4524 J/bar 44.524 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CUBIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = -3.5580 \times 10^3 + 3.3473 \times 10^2 T^{0.5} - 9.3090 T + 2.5388 \times 10^{-3} T^2$$

$$+ 1.4273 \times 10^5 T^{-1}$$

(EQUATION VALID FROM 298 - 848 K)

$$C_P^0 = 96.823 + 5.2733 \times 10^{-2} T + 5.6413 \times 10^{-7} T^{-2}$$

(EQUATION VALID FROM 848 - 1800 K)

REFERENCE	44	79	84	COMPILED
	79		247	6-11-76

GALLIUM SESQUIOXIDE

FORMULA WEIGHT 187.438

Ga<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP.						FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>	
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	84.98	84.98	92.13	-1089.100	-998.342	174.906	
UNCERTAINTY		0.42	0.42		0.850	0.850	0.149	
-----								
400	25.050	113.82	88.77	103.63	-1100.416	-963.710	125.848	
500	41.520	137.75	96.23	110.66	-1099.664	-929.604	97.115	
600	53.475	158.38	104.90	115.56	-1098.425	-895.694	77.977	
700	62.616	176.48	113.86	119.21	-1096.879	-862.029	64.326	
800	69.872	192.59	122.72	122.04	-1095.124	-828.592	54.102	
900	75.800	207.10	131.30	124.30	-1093.217	-795.380	46.163	
1000	80.745	220.29	139.55	126.16	-1091.192	-762.392	39.823	
-----								
1100	84.945	232.39	147.44	127.71	-1089.074	-729.627	34.647	
1200	88.565	243.56	155.00	129.02	-1086.879	-697.029	30.341	
1300	91.721	253.93	162.21	130.14	-1084.620	-664.629	26.705	
1400	94.500	263.62	169.12	131.10	-1082.307	-632.431	23.596	
1500	96.969	272.69	175.72	131.94	-1079.942	-600.377	20.907	
1600	99.178	281.23	182.05	132.67	-1077.538	-568.506	18.560	
1700	101.168	289.29	188.12	133.32	-1075.094	-536.764	16.493	
1800	102.969	296.93	193.96	133.88	-1072.619	-505.151	14.659	

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	2.8941 J/bar 28.941 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

GALLIUM.... M. P. 302.9 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.6578 \times 10^2 - 2.4571 \times 10^{-3} T - 1.1589 \times 10^3 T^{-0.5} - 5.1563 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	203	120	262	COMPILED
			145	6- 2-76

## GADOLINIUM SESQUIOXIDE (MONOCLINIC)

FORMULA WEIGHT 362.498

Gd<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	151.88	151.88	109.54	-1819.620	-1732.338	303.500
UNCERTAINTY		0.85	0.85		3.600	3.600	0.631
400	28.025	184.82	156.79	114.48	-1819.248	-1702.831	222.368
500	45.644	210.73	165.09	117.69	-1817.862	-1673.897	174.872
600	57.867	232.42	174.55	120.20	-1816.452	-1645.138	143.223
700	66.927	251.11	184.18	122.35	-1815.113	-1616.684	120.639
800	73.977	267.58	193.60	124.29	-1813.860	-1588.428	103.714
900	79.667	282.32	202.65	126.09	-1812.693	-1560.306	90.558
1000	84.399	295.70	211.30	127.81	-1811.596	-1532.392	80.044
1100	88.421	307.96	219.54	129.47	-1810.577	-1504.432	71.440
1200	91.909	319.29	227.38	131.07	-1809.668	-1476.696	64.279
1300	94.982	329.85	234.87	132.64	-1808.874	-1448.998	58.222
1400	97.729	339.73	242.00	134.19	-1808.219	-1421.248	53.028
1500	100.209	349.04	248.83	135.71	-1807.706	-1393.607	48.530
1600	102.475	357.85	255.38	137.21	-1834.143	-1365.633	44.584
1700	104.562	366.21	261.65	138.70	-1833.328	-1336.356	41.061
1800	106.499	374.18	267.68	140.17	-1832.399	-1307.105	37.931

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.3400 J/bar 43.400 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

GADOLINIUM. ALPHA-BETA 1533, M. P. 1585 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 1.1925 \times 10^2 + 1.3585 \times 10^{-2} T - 1.4351 \times 10^2 T^{-0.5} - 4.8486 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	210	281	235	COMPILED 5-18-76
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GADOLINIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 362.498

Gd<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1500 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$\frac{S_T^0}{S_{298}^0} -$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS		
					ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log $f$
298.15	0.000	0.00	---	116.87	---	---	---
UNCERTAINTY							
400	28.100	34.12	---	116.41	---	---	---
500	46.010	60.37	---	119.13	---	---	---
600	58.455	82.36	---	122.21	---	---	---
700	67.767	101.42	---	125.02	---	---	---
800	75.079	118.27	---	127.43	---	---	---
900	81.011	133.40	---	129.44	---	---	---
1000	85.941	147.13	---	131.11	---	---	---
1100	90.112	159.69	---	132.48	---	---	---
1200	93.691	171.27	---	133.59	---	---	---
1300	96.796	182.00	---	134.49	---	---	---
1400	99.514	192.00	---	135.19	---	---	---
1500	101.913	201.34	---	135.74	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.7585 J/bar 47.585 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

GADOLINIUM. ALPHA-BETA 1533, M. P. 1585 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 2.0401 \times 10^2 - 1.1112 \times 10^{-2} T - 2.0523 \times 10^3 T^{-0.5} + 3.1138 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE 210

COMPILED  
5-18-76

## GERMANIUM DIOXIDE (QUARTZ TYPE)

FORMULA WEIGHT 104.589

GeO<sub>2</sub>: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	55.27	55.27	52.09	-551.030	-497.074	87.086
UNCERTAINTY		0.27	0.27		0.800	0.900	0.158
400	14.125	71.54	57.41	58.61	-550.844	-478.664	62.507
500	23.524	85.15	61.63	63.33	-550.261	-460.676	48.127
600	30.463	97.02	66.56	66.83	-549.417	-442.833	38.552
700	35.854	107.52	71.67	69.46	-548.395	-425.146	31.725
800	40.184	116.93	76.75	71.45	-547.258	-407.610	26.614
900	43.744	125.44	81.70	72.98	-546.058	-390.223	22.648
1000	46.730	133.19	86.46	74.14	-544.833	-372.973	19.482
1100	49.263	140.30	91.04	75.01	-543.627	-355.846	16.898
1200	51.437	146.86	95.42	75.66	-542.469	-338.829	14.749
1300	53.318	152.93	99.61	76.12	-578.190	-319.178	12.825

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.4440 J/bar 24.440 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

GERMANIUM.. M. P. 1210.4 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.2667 \times 10^2 - 1.0156 \times 10^{-2} T - 1.3604 \times 10^3 T^{-0.5} + 6.4330 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1350 K)

REFERENCE	119	120	262	COMPILED
			83	6- 8-76



GERMANIUM DIOXIDE GLASS

FORMULA WEIGHT 104.589

GeO<sub>2</sub>: Glass 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	64.50	64.50	44.38	-526.350	-475.180	83.250
UNCERTAINTY		0.30	0.30		0.630	0.710	0.124
400	14.250	79.67	65.42	57.70	-526.114	-457.186	59.703
500	23.646	93.31	69.66	64.14	-525.520	-440.015	45.968
600	30.738	105.37	74.63	67.98	-524.572	-422.998	36.825
700	36.253	116.05	79.80	70.55	-523.436	-406.158	30.308
800	40.664	125.60	84.94	72.45	-522.194	-389.482	25.431
900	44.278	134.22	89.94	73.94	-520.898	-372.965	21.646
1000	47.310	142.08	94.77	75.17	-519.573	-356.603	18.627
1100	49.893	149.29	99.40	76.23	-518.254	-340.362	16.163
1200	52.127	155.97	103.84	77.17	-516.960	-324.252	14.114
1300	54.088	162.18	108.09	78.03	-552.510	-305.523	12.276
1400	55.829	167.99	112.16	78.82	-551.046	-286.572	10.692
1500	57.384	173.45	116.07	79.56	-549.542	-267.722	9.323
1600	58.792	178.61	119.82	80.26	-547.989	-248.997	8.129
1700	60.075	183.50	123.43	80.94	-546.391	-230.378	7.079
1800	61.252	188.14	126.89	81.59	-544.748	-211.820	6.147

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	J/bar

GERMANIUM.. M. P. 1210.4 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 76.125 + 4.8606 \times 10^{-3} T - 1.0814 \times 10^{-5} T^2 + 2.3943 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	119	163	COMPILED 5-28-76
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WATER FORMULA WEIGHT 18.015

H<sub>2</sub>O: Liquid 298.15 to 372.8 K. Ideal gas 372.8 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	69.95	69.95	75.19	-285.830	-237.141	41.546
UNCERTAINTY		0.08	0.08		0.042	0.084	0.015
372.8	15.216	86.76	71.63	75.89	-283.703	-225.106	31.541
372.8	124.836	196.38	71.63	34.09	-242.437	-225.106	31.541
400	118.672	198.78	80.11	34.28	-242.836	-223.882	29.236
500	101.882	206.53	104.65	35.18	-243.820	-219.035	22.883
600	90.853	213.04	122.19	36.26	-244.758	-213.987	18.629
700	83.139	218.71	135.57	37.45	-245.634	-208.786	15.580
800	77.506	223.80	146.29	38.70	-246.444	-203.473	13.285
900	73.266	228.43	155.16	39.97	-247.185	-198.045	11.494
1000	69.999	232.71	162.71	41.24	-247.859	-192.559	10.058
1100	67.442	236.69	169.25	42.48	-248.464	-186.985	8.879
1200	65.412	240.44	175.03	43.69	-249.008	-181.371	7.895
1300	63.786	243.99	180.20	44.85	-249.492	-175.730	7.061
1400	62.473	247.35	184.88	45.95	-249.923	-170.040	6.344
1500	61.406	250.56	189.15	46.98	-250.303	-164.322	5.722
1600	60.535	253.62	193.08	47.96	-250.640	-158.569	5.177
1700	59.822	256.55	196.73	48.85	-250.937	-152.805	4.695
1800	59.236	259.37	200.13	49.68	-251.201	-147.035	4.267

MELTING POINT	273.15 K	BOILING POINT	372.8 K
ENTHALPY OF MELTING	6.008 kJ	ENTHALPY OF VAPOORIZATION	40.866 kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	13.293 kJ	MOLAR VOLUME	1.8069 J/bar 18.069 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

#### HEAT CAPACITY EQUATION

$$C_P^0 = 7.3680 + 2.7468 \times 10^{-2} T - 4.8117 \times 10^{-6} T^2 + 3.6174 \times 10^{-9} T^3 - 2.2316 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 372.8 - 1800 K)

REFERENCE	247 196	35	35	COMPILED 8-03-76
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STEAM

FORMULA WEIGHT 18.015

H<sub>2</sub>O: Ideal gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	188.83	188.83	33.58	-241.814	-228.569	40.044
UNCERTAINTY		0.04	0.04		0.042	0.084	0.015
400	8.630	198.78	190.15	34.28	-242.837	-223.883	29.236
500	13.840	206.52	192.68	35.18	-243.825	-219.035	22.883
600	17.497	213.03	195.54	36.26	-244.756	-213.981	18.629
700	20.263	218.72	198.45	37.45	-245.631	-208.788	15.580
800	22.489	223.80	201.31	38.70	-246.442	-203.471	13.285
900	24.360	228.43	204.07	39.97	-247.184	-198.042	11.494
1000	25.978	232.70	206.72	41.24	-247.864	-192.557	10.058
1100	27.425	236.69	209.27	42.48	-248.467	-186.989	8.879
1200	28.730	240.44	211.71	43.69	-249.011	-181.374	7.895
1300	29.925	243.98	214.06	44.85	-249.495	-175.724	7.061
1400	31.034	247.35	216.31	45.95	-249.922	-170.034	6.344
1500	32.063	250.56	218.49	46.98	-250.301	-164.316	5.722
1600	33.027	253.62	220.59	47.96	-250.636	-158.564	5.177
1700	33.932	256.56	222.62	48.85	-250.933	-152.812	4.695
1800	34.783	259.37	224.59	49.68	-251.201	-147.032	4.267

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	9.908 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

HEAT CAPACITY EQUATION

$$C_P^0 = 7.3680 + 2.7468 \times 10^{-2} T - 4.8117 \times 10^{-6} T^2 + 3.6174 \times 10^{-9} T^3 - 2.2316 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	35	35	COMPILED
	196		196	8-17-76

## HAFNIA

FORMULA WEIGHT 210.489

HfO<sub>2</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	59.33	59.33	60.25	-1144.740	-1088.276	190.662
UNCERTAINTY		0.42	0.42		1.255	1.297	0.227
400	16.275	78.06	61.78	66.91	-1143.912	-1069.100	139.611
500	26.828	93.45	66.62	70.94	-1142.763	-1050.528	109.748
600	34.427	106.65	72.22	73.77	-1141.453	-1032.199	89.861
700	40.209	118.19	77.98	75.93	-1140.061	-1014.103	75.674
800	44.785	128.45	83.66	77.65	-1138.630	-996.206	65.046
900	48.522	137.68	89.16	79.09	-1137.180	-978.483	56.790
1000	51.639	146.08	94.44	80.32	-1135.736	-960.936	50.194
1100	54.296	153.78	99.48	81.39	-1134.300	-943.516	44.804
1200	56.595	160.91	104.32	82.35	-1132.882	-926.242	40.318
1300	58.609	167.53	108.92	83.21	-1131.488	-909.071	36.527
1400	60.393	173.73	113.34	83.99	-1130.124	-892.026	33.282
1500	61.993	179.55	117.56	84.72	-1128.785	-875.060	30.472
1600	63.434	185.04	121.61	85.39	-1127.483	-858.187	28.017
1700	64.744	190.23	125.49	86.02	-1126.216	-841.398	25.853
1800	65.943	195.17	129.23	86.61	-1124.987	-824.693	23.932

MELTING POINT	3173	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.0823 J/bar 20.823 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS				

HAFNIUM.... ALPHA-BETA 2013 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 95.584 + 2.0947 \times 10^{-3} T - 5.3496 \times 10^{-6} T^{0.5} - 4.4246 \times 10^{-9} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	188	120	264	COMPILED 5-26-76
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MONTROYDITE

FORMULA WEIGHT 216.589

HgO: Crystals 298.15 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	70.27	70.27	44.06	-90.789	-58.528	10.254
UNCERTAINTY		0.34	0.34		0.050	0.060	0.011
400	11.825	83.89	72.06	48.53	-90.388	-47.558	6.210
500	19.488	95.06	75.57	51.60	-89.633	-36.928	3.858
600	25.043	104.69	79.65	53.95	-88.647	-26.478	2.305
700	29.313	113.15	83.84	55.84	-146.260	-9.550	0.713
800	32.731	120.71	87.98	57.43	-144.338	9.853	-0.643
900	35.556	127.56	92.00	58.79	-142.301	29.009	-1.683
1000	37.938	133.82	95.88	60.00	-140.170	47.926	-2.503

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	9.113 kJ	MOLAR VOLUME	1.9320 J/bar 19.320 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MERCURY.... B. P. 629 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 73.566 + 3.0351 \times 10^{-3} T - 5.2510 \times 10^{-2} T^{-0.5}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	247	247	258	COMPILED
			247	6- 9-76

## HOLMIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 377.859

Ho<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	158.16	158.16	106.86	-1880.700	-1791.373	313.842
UNCERTAINTY		0.32	0.32		4.850	5.000	0.876
400	29.400	191.51	162.11	118.61	-1879.106	-1760.876	229.948
500	47.762	218.53	170.77	123.13	-1877.175	-1731.535	180.893
600	60.532	241.20	180.67	125.43	-1875.093	-1702.602	148.225
700	69.916	260.65	190.73	126.93	-1873.017	-1674.014	124.917
800	77.120	277.68	200.56	128.15	-1871.040	-1645.732	107.456
900	82.856	292.84	209.98	129.30	-1869.229	-1617.652	93.886
1000	87.557	306.53	218.97	130.47	-1867.648	-1589.808	83.043
1100	91.513	319.02	227.51	131.69	-1866.352	-1562.092	74.178
1200	94.913	330.53	235.62	132.97	-1865.401	-1534.459	66.794
1300	97.892	341.23	243.34	134.32	-1864.847	-1506.918	60.549
1400	100.543	351.23	250.69	135.74	-1864.753	-1479.403	55.197
1500	102.941	360.65	257.71	137.22	-1865.169	-1451.844	50.558
1600	105.131	369.55	264.42	138.76	-1866.162	-1424.266	46.498
1700	107.155	378.01	270.86	140.34	-1867.792	-1396.612	42.913
1800	109.044	386.08	277.04	141.98	-1900.495	-1367.605	39.687

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	21.004 kJ	MOLAR VOLUME	4.4900 J/bar 44.900 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

HOLMIUM.... ALPHA-BETA 1701, M. P. 1743 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 74.141 + 2.2966 \times 10^{-2} T + 1.1732 \times 10^{-5} T^{0.5} - 3.7399 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	207	235	235	COMPILED 5-19-76
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DIPOTASSIUM MONOXIDE FORMULA WEIGHT 94.195

K<sub>2</sub>O: Crystals 298.15 to 1800 K. Decomposes above 1154 K. Tabulated data are a metastable extrapolation for temperatures greater than 1154 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	94.14	94.14	83.68	-363.171	-322.087	56.429
UNCERTAINTY		6.28	6.28		2.092	2.845	0.498
400	22.200	119.72	97.52	90.13	-366.867	-307.317	40.132
500	36.240	140.32	104.08	94.47	-365.379	-292.584	30.566
600	46.268	157.89	111.62	98.31	-363.394	-278.215	24.221
700	53.969	173.32	119.35	102.03	-360.992	-264.196	19.715
800	60.209	187.19	126.98	105.77	-358.227	-250.551	16.359
900	65.478	199.86	134.38	109.56	-355.142	-237.269	13.771
1000	70.083	211.61	141.53	113.43	-351.751	-224.351	11.779
1100	74.202	222.60	148.40	117.36	-506.535	-203.151	9.647
1200	77.964	232.98	155.02	121.35	-500.535	-175.835	7.654
1300	81.457	242.86	161.40	125.40	-494.149	-149.042	5.989
1400	84.743	252.30	167.56	129.49	-487.371	-122.730	4.579
1500	87.863	261.37	173.51	133.63	-480.200	-96.926	3.375
1600	90.854	270.13	179.28	137.80	-472.625	-71.635	2.339
1700	93.739	278.61	184.87	142.01	-464.641	-46.800	1.438
1800	96.538	286.85	190.31	146.25	-456.250	-22.439	0.651

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.0380 J/bar 40.380 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 49.265 + 4.6059 \times 10^{-2} T + 6.1447 \times 10^{-5} T^{-0.5} - 1.3249 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	247	247	COMPILED 5-24-76
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POTASSIUM SUPEROXIDE FORMULA WEIGHT 71.097

KO<sub>2</sub>: Crystals 298.15 to melting point 782 K. Above 782 K the data tabulated are a metastable extrapolation.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS								
	$(H_T^0 - H_{298}^0)/T$		$S_T^0$	$-(G_T^0 - H_{298}^0)/T$		$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	122.50	122.50	77.53	-284.512	-240.586	42.150		
UNCERTAINTY		4.18	4.18		2.092	2.800	0.491		
400	20.600	146.24	125.64	83.80	-284.828	-225.444	29.440		
500	33.656	165.38	131.72	87.59	-282.414	-210.864	22.029		
600	42.870	181.59	138.72	90.13	-279.721	-196.807	17.134		
700	49.759	195.63	145.87	91.93	-276.861	-183.215	13.672		
800	55.116	207.99	152.87	93.24	-273.910	-170.030	11.102		
900	59.411	219.03	159.62	94.19	-270.921	-157.215	9.125		
1000	62.923	229.00	166.08	94.89	-267.941	-144.751	7.561		
1100	65.854	238.06	172.21	95.40	-344.216	-128.251	6.090		
1200	68.332	246.38	178.05	95.75	-340.287	-108.796	4.736		
1300	70.451	254.06	183.61	95.98	-336.365	-89.672	3.603		
1400	72.279	261.17	188.89	96.12	-332.461	-70.831	2.643		
1500	73.871	267.81	193.94	96.17	-328.573	-52.283	1.821		

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.2840 J/bar 32.840 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. H. P. 336.4, B. P. 1030 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 125.95 - 6.5626 \times 10^{-3} T - 769.25 T^{-0.5} - 1.7033 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	32	32	32	COMPILED
	204			6- 8-76



POTASSIUM HYDROXIDE

FORMULA WEIGHT 56.105

KOH: Crystals 298.15 to melting point 679 K. Liquid 679 to boiling point 1596 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	78.91	78.91	64.89	-424.676	-378.932	66.388
UNCERTAINTY		0.84	0.84		0.418	0.500	0.088
400	17.362	98.90	81.53	71.67	-426.256	-362.863	47.385
500	28.996	115.72	86.72	79.58	-424.807	-347.163	36.268
600	48.053	142.59	94.54	78.66	-416.556	-332.859	28.978
679	51.614	183.30	131.68	78.66	-415.145	-342.931	26.381
679	64.308	195.99	131.68	83.11	-406.526	-342.931	26.381
700	64.871	198.33	133.46	83.11	-406.066	-340.865	25.436
800	67.150	209.47	142.32	83.11	-403.877	-331.733	21.660
900	68.924	219.25	150.33	83.11	-401.741	-322.829	18.737
1000	70.342	228.00	157.66	83.11	-399.679	-314.169	16.411
1100	71.503	235.91	164.41	83.11	-476.926	-301.386	14.312
1200	72.470	243.14	170.67	83.11	-474.009	-285.556	12.430
1300	73.288	249.79	176.50	83.11	-471.130	-269.970	10.848
1400	73.989	249.79	175.80	83.11	-468.288	-245.977	9.178
1500	74.597	255.95	181.35	83.11	-465.483	-230.833	8.038

MELTING POINT	679 K	BOILING POINT	1596 K
ENTHALPY OF MELTING	8.619 kJ	ENTHALPY OF VAPORIZATION	142.700 kJ
$H_{298}^0 - H_0^0$	12.163 kJ	MOLAR VOLUME	2.7450 J/bar 27.450 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

REFERENCE	709	709	709	COMPILED 10-11-74
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## LANTHANUM SESQUIOXIDE

FORMULA WEIGHT 325.809

La<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	127.32	127.32	107.95	-1793.680	-1705.963	298.879
UNCERTAINTY		0.84	0.84		1.590	1.600	0.280
400	28.700	160.38	131.68	116.51	-1792.296	-1676.190	218.889
500	46.776	186.93	140.15	121.33	-1790.480	-1647.370	172.100
600	59.495	209.37	149.87	124.68	-1789.155	-1618.878	140.936
700	68.999	228.79	159.79	127.28	-1787.113	-1590.658	118.697
800	76.422	245.93	169.51	129.44	-1785.198	-1562.730	102.036
900	82.422	261.29	178.87	131.34	-1783.437	-1535.901	89.142
1000	87.400	275.21	187.81	133.07	-1781.875	-1507.495	78.744
1100	91.625	287.97	196.35	134.66	-1780.503	-1480.126	70.286
1200	95.274	299.75	204.48	136.17	-1778.434	-1452.420	63.222
1300	98.475	310.71	212.23	137.61	-1776.987	-1423.640	57.203
1400	101.321	320.96	219.64	138.99	-1795.449	-1394.993	52.048
1500	103.877	330.59	226.71	140.34	-1793.821	-1366.426	47.583
1600	106.196	339.69	233.49	141.65	-1792.099	-1338.011	43.682
1700	108.319	348.32	240.00	142.93	-1790.282	-1309.701	40.242
1800	110.277	356.52	246.24	144.19	-1788.371	-1281.473	37.188

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	19.841 kJ	MOLAR VOLUME	4.9560 J/bar 49.560 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

LANTHANUM.. ALPHA-BETA 550, BETA-GAMMA 1134, M. P. 1193 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.3102 \times 10^2 + 1.0576 \times 10^{-2} T - 2.3418 \times 10^{-5} T^2 - 1.1252 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	142	235	235	COMPILED 5-18-76
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LITHIUM MONOXIDE FORMULA WEIGHT 29.879

Li<sub>2</sub>O: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	37.57	37.57	54.09	-598.730	-561.985	98.458
UNCERTAINTY		0.08	0.08		2.092	2.134	0.374
400	14.975	54.79	39.82	62.99	-599.576	-549.294	71.731
500	25.236	69.55	44.31	69.26	-606.314	-536.024	55.998
600	32.992	82.62	49.63	74.09	-606.667	-521.926	45.438
700	39.150	94.35	55.20	78.00	-606.544	-507.809	37.893
800	44.216	104.98	60.76	81.27	-606.048	-493.724	32.237
900	48.489	114.72	66.23	84.08	-605.259	-479.736	27.843
1000	52.178	123.71	71.53	86.55	-604.209	-465.849	24.334
1100	55.405	132.07	76.67	88.75	-602.949	-452.062	21.467
1200	58.268	139.87	81.60	90.74	-601.497	-438.399	19.083
1300	60.837	147.21	86.37	92.56	-599.872	-424.879	17.072
1400	63.164	154.13	90.97	94.24	-598.089	-411.483	15.353
1500	65.289	160.69	95.40	95.81	-596.154	-398.229	13.868
1600	67.243	166.92	99.68	97.28	-594.075	-385.107	12.573
1700	69.051	172.86	103.81	98.67	-881.909	-357.636	10.989

MELTING POINT	1700	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	11.401	kJ	MOLAR VOLUME	1.4760 J/bar 14.760 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LITHIUM.... M. P. 453.69, B. P. 1618 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.1748 \times 10^2 + 5.3302 \times 10^{-3} T - 1.1515 \times 10^3 T^{-0.5} + 1.5180 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 247      247      247      COMPILED 5-24-76

LITHIUM HYDROXIDE FORMULA WEIGHT 23.947

LiOH: Crystals 298.15 to melting point 744.3 K. Liquid 744.3 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	42.80	42.80	49.59	-484.926	-438.941	76.901
UNCERTAINTY		0.21	0.21		0.159	0.159	0.028
400	13.800	58.66	44.86	58.04	-485.061	-423.193	55.264
500	23.230	72.24	49.01	63.64	-487.877	-407.440	42.565
600	30.355	84.26	53.91	68.20	-487.299	-391.401	34.075
700	36.056	95.08	59.02	72.28	-486.297	-375.491	28.020
744.30	38.231	100.13	61.90	73.99	-485.742	-368.832	25.885
744.30	66.281	128.18	61.90	86.78	-464.864	-368.832	25.885
800	67.729	133.89	66.16	86.78	-463.398	-361.350	23.594
900	69.878	144.14	74.26	86.78	-460.767	-348.744	20.241
1000	71.546	153.26	81.71	86.78	-458.222	-336.442	17.574

MELTING POINT	744.30 K	BOILING POINT	K
ENTHALPY OF MELTING	20.878 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	7.414 kJ	MOLAR VOLUME	1.6440 J/bar 16.440 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LITHIUM.... M. P. 453.69, B. P. 1618 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 51.051 + 3.3271 \times 10^{-2} T - 1.0116 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 744.30 K)

REFERENCE	32	215	215	COMPILED 5-19-76
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LUTETIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 397.938

Lu<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	109.96	109.96	96.39	-1878.200	-1788.849	313.400
UNCERTAINTY		0.85	0.85		7.530	6.280	1.100
400	26.725	140.34	113.61	109.39	-1877.510	-1758.252	229.605
500	43.996	165.54	121.54	116.15	-1876.178	-1728.583	180.585
600	56.398	187.12	130.72	120.38	-1874.499	-1699.212	147.930
700	65.759	205.91	140.15	123.29	-1872.679	-1670.148	124.629
800	73.090	222.51	149.42	125.43	-1870.842	-1641.334	107.169
900	79.000	237.39	158.39	127.09	-1869.073	-1612.753	93.602
1000	83.879	250.85	166.97	128.41	-1867.428	-1584.348	82.758
1100	87.978	263.14	175.16	129.50	-1865.966	-1556.118	73.894
1200	91.478	274.45	182.97	130.42	-1864.731	-1528.005	66.513
1300	94.505	284.92	190.42	131.20	-1863.761	-1499.995	60.271
1400	97.150	294.67	197.52	131.88	-1863.097	-1472.035	54.923
1500	99.487	303.79	204.30	132.48	-1862.769	-1444.104	50.288
1600	101.567	312.36	210.79	133.02	-1862.816	-1416.200	46.234
1700	103.431	320.44	217.01	133.49	-1863.270	-1388.299	42.657
1800	105.113	328.08	222.97	133.92	-1864.162	-1360.324	39.476

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	17.539 kJ	MOLAR VOLUME	4.2220 J/bar 42.220 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LUTETIUM... M. P. 1936 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.4705 \times 10^2 - 5.3393 \times 10^2 T^{-0.5} - 1.7548 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	202	281	235	COMPILED
				6- 8-76

PERICLASE FORMULA WEIGHT 40.304

HgO: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	26.94	26.94	37.78	-601.490	-569.196	99.721
UNCERTAINTY		0.17	0.17		0.290	0.300	0.053
400	10.250	38.72	28.47	42.45	-601.501	-558.147	72.887
500	17.010	48.55	31.54	45.41	-601.302	-547.337	57.180
600	21.908	57.00	35.09	47.36	-601.031	-536.564	46.712
700	25.634	64.40	38.77	48.74	-600.762	-525.848	39.239
800	28.580	70.96	42.38	49.78	-600.528	-515.157	33.636
900	30.978	76.87	45.89	50.59	-600.351	-504.492	29.280
1000	32.974	82.24	49.27	51.23	-609.192	-493.092	25.757
1100	34.665	87.15	52.49	51.76	-609.051	-481.484	22.864
1200	36.116	91.68	55.56	52.19	-608.882	-469.892	20.454
1300	37.375	95.88	58.50	52.55	-608.689	-458.319	18.416
1400	38.479	99.80	61.32	52.85	-735.442	-443.164	16.535
1500	39.446	103.45	64.00	53.09	-734.047	-422.331	14.707
1600	40.302	106.88	66.58	53.32	-732.649	-401.586	13.110
5000	41.059	110.11	69.05	53.50	-731.261	-380.951	11.705
1800	41.729	113.14	71.41	53.66	-729.887	-360.383	10.458

MELTING POINT	3125	K	BOILING POINT		K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION		kJ
$H_{298}^0 - H_0^0$	5.166	kJ	MOLAR VOLUME	1.1248	J/bar
				11.248	cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. N. P. 922, B. P. 1361 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 65.211 - 1.2699 \times 10^{-3} T - 387.24 T^{-0.5} - 4.6185 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	261	215	215	COMPILED
	204		247	7-15-76

BRUCITE FORMULA WEIGHT 58.320

Mg(OH)<sub>2</sub>: Crystals 298.15 to 900 K. At approximately 540 K the partial pressure of steam in equilibrium with brucite reaches one atmosphere.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>p</sub> <sup>o</sup> J/mol·K			
298.15	0.000	63.18	63.18	77.28	-924.540	-833.506	146.027
UNCERTAINTY		0.13	0.13		0.440	0.440	0.077
400	21.775	88.21	66.43	91.91	-924.416	-802.310	104.771
500	36.612	109.59	72.98	99.30	-923.482	-771.901	80.640
600	47.477	128.14	80.66	104.01	-922.180	-741.712	64.572
700	55.810	144.44	88.63	107.45	-920.691	-711.766	53.113
800	62.442	158.98	96.54	110.22	-919.108	-682.042	44.533
900	67.889	172.10	104.21	112.59	-917.475	-652.494	37.870

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	11.401 kJ	MOLAR VOLUME	2.4630 J/bar 24.630 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. H. P. 922, B. P. 1361 K.

HEAT CAPACITY EQUATION

$$C_p^o = 1.0222 \times 10^2 + 1.5107 \times 10^{-2} T - 2.6172 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	131	214	214	COMPILED
			102	5-26-76

## MANGANOSITE

FORMULA WEIGHT 70.937

MnO: Crystals 298.15 to melting point 2054 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS							
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	59.71	59.71	44.10	-385.220	-362.896	63.578	
UNCERTAINTY		0.42	0.42		0.460	0.502	0.088	
400	11.600	73.08	61.48	46.86	-384.870	-355.324	46.401	
500	18.856	83.76	64.90	48.78	-384.538	-347.978	36.353	
600	23.973	92.79	68.82	50.28	-384.268	-340.693	29.660	
700	27.823	100.63	72.81	51.52	-384.073	-333.442	24.882	
800	30.854	107.59	76.74	52.59	-383.955	-326.223	21.300	
900	33.322	113.83	80.51	53.53	-383.905	-318.997	18.514	
1000	35.386	119.52	84.13	54.38	-386.141	-311.751	16.284	
1100	37.148	124.74	87.59	55.16	-386.207	-304.312	14.451	
1200	38.680	129.57	90.89	55.89	-386.261	-296.855	12.922	
1300	40.030	134.07	94.04	56.57	-386.306	-289.404	11.628	
1400	41.236	138.29	97.05	57.22	-388.624	-281.888	10.517	
1500	42.321	142.26	99.94	57.84	-391.116	-274.131	9.546	
1600	43.309	146.01	102.70	58.43	-403.802	-265.650	8.673	
1700	44.216	149.57	105.35	59.00	-404.382	-257.001	7.897	
1800	45.053	152.96	107.91	59.56	-404.918	-248.318	7.206	

MELTING POINT	2054	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	1.3221 J/bar 13.221 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 59.749 + 3.6000 \times 10^{-3} T - 2.8265 \times 10^{-6} T^2 - 3.1362 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	242	120	263	COMPILED 6-8-76
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PYROLUSITE

FORMULA WEIGHT 86.937

MnO<sub>2</sub>: Crystals 298.15 to 800 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	53.05	53.05	54.02	-520.030	-465.138	81.491
UNCERTAINTY		0.42	0.42		0.837	0.879	
400	15.125	70.45	55.32	63.53	-519.782	-446.410	58.295
500	25.314	85.17	59.86	68.08	-519.163	-428.133	44.727
600	32.692	97.84	65.15	70.89	-518.473	-409.987	35.693
700	38.300	108.93	70.63	72.93	-517.803	-391.964	29.249
800	42.735	118.78	76.05	74.60	-517.180	-374.028	24.422

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	1.6610 J/bar 16.610 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 57.665 + 1.3383 \times 10^{-2} T + 2.6688 \times 10^{-5} T^{-0.5} - 2.0526 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 800 K)

REFERENCE	168	120	263	COMPILED 6-14-76
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## BIIBYITE

FORMULA WEIGHT 157.874

Mn<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	110.46	110.46	107.65	-958.970	-881.068	154.360
UNCERTAINTY		2.09	2.09		2.092	2.218	0.389
400	27.475	142.15	114.67	109.02	-958.072	-854.602	111.600
500	44.204	166.93	122.73	113.55	-957.404	-828.814	86.586
600	56.203	188.10	131.90	118.90	-956.738	-803.159	69.922
700	65.547	206.84	141.29	124.29	-955.999	-777.625	58.027
800	73.211	223.77	150.56	129.37	-955.157	-752.194	49.113
900	79.711	239.28	159.57	133.99	-954.199	-726.868	42.186
1000	85.349	253.62	168.27	138.08	-957.582	-701.592	36.648
1100	90.306	266.94	176.63	141.58	-956.433	-676.042	32.103
1200	94.703	279.39	184.69	144.46	-955.115	-650.598	28.320
1300	98.622	291.05	192.43	146.71	-953.681	-625.289	25.125

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.1370 J/bar 31.370 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 61.943 + 0.10847 T - 3.3789 \times 10^{-5} T^2 + 1.4552 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	115	120	263	COMPILED
	191		197	6-14-76

HAUSMANNITE

FORMULA WEIGHT 228.812

Mn<sub>3</sub>O<sub>4</sub>: Tetragonal crystals 298.15 to 1445 K. Cubic crystals 1445 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	153.97	153.97	139.29	-1387.830	-1282.774	224.738
UNCERTAINTY		4.18	4.18		1.674	2.092	0.367
400	39.175	199.01	159.83	162.60	-1386.542	-1247.038	162.847
500	64.484	235.98	171.50	167.73	-1384.870	-1212.365	126.655
600	81.855	266.73	184.88	169.57	-1383.639	-1177.989	102.553
700	94.527	293.02	198.49	171.69	-1382.903	-1143.783	85.351
800	104.367	316.15	211.78	175.03	-1382.511	-1109.647	72.453
900	112.467	337.02	224.55	179.74	-1382.254	-1075.534	62.423
1000	119.486	356.26	236.77	185.73	-1388.612	-1041.352	54.395
1100	125.825	374.29	248.47	192.86	-1388.073	-1006.659	47.802
1200	131.743	391.41	259.67	200.99	-1386.984	-972.000	42.310
1300	137.411	407.85	270.44	209.97	-1385.241	-937.495	37.669
1400	142.936	423.67	280.73	219.70	-1389.601	-902.821	33.685
1445	145.172	430.45	285.28	224.30	-1394.952	-887.166	32.070
1445	159.047	444.33	285.28	210.04	-1374.903	-887.166	32.070
1500	160.917	451.79	290.87	210.04	-1374.893	-867.888	30.223
1600	163.986	465.34	301.36	210.04	-1411.227	-832.112	27.166
1700	166.695	478.06	311.37	210.04	-1411.429	-795.898	24.455
1800	169.103	490.11	321.01	210.04	-1411.678	-759.758	22.048

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	4.6950 J/bar 46.950 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -2.4065 \times 10^2 + 0.17137 T + 8.5280 \times 10^3 T^{-0.5} - 1.4672 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 298 - 1445 K)

REFERENCE	241	197	263 197	COMPILED 6- 8-76
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## MOLYBDENUM DIOXIDE

FORMULA WEIGHT 127.939

MoO<sub>2</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	50.02	50.02	55.90	-587.850	-533.053	93.389
UNCERTAINTY		0.30	0.30		2.090	2.510	0.440
400	15.400	67.72	52.32	63.88	-587.218	-514.406	67.175
500	25.530	82.46	56.93	68.02	-586.222	-496.327	51.851
600	32.873	95.13	62.26	71.04	-585.035	-478.445	41.653
700	38.517	106.29	67.77	73.69	-583.713	-460.793	34.385
800	43.072	116.29	73.22	76.23	-582.260	-443.324	28.946
900	46.900	125.42	78.52	78.76	-580.668	-426.048	24.727
1000	50.212	133.85	83.64	81.33	-578.933	-408.963	21.362
1100	53.159	141.72	88.56	126.95	-577.041	-392.054	18.617
1200	55.835	149.14	93.31	126.95	-574.987	-375.331	16.338
1300	58.306	156.18	97.87	126.95	-572.764	-358.784	14.416
1400	60.621	162.90	102.28	126.95	-570.368	-342.406	12.775
1500	62.811	169.35	106.54	126.95	-567.800	-326.225	11.360
1600	64.903	175.56	110.66	126.95	-565.055	-310.207	10.127
1700	66.918	181.57	114.65	126.95	-562.133	-294.366	9.045
1800	68.870	187.40	118.53	126.95	-559.035	-278.703	8.088

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	1.9580 J/bar 19.580 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MOLYBDENUM. M. P. 2890 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 27.146 + 3.3248 \times 10^{-2} T + 7.2748 \times 10^{-5} T^{-0.5} - 2.0703 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1074 K)

REFERENCE	247	247	247	COMPILED
	140		159	5-24-76

HOLYBDITE

FORMULA WEIGHT 143.938

MoO<sub>3</sub>: Crystals 298.15 to melting point 1074 K. Liquid 1074 to 1500 K.

TEMP. K	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	77.74	77.74	74.88	-745.170	-668.055	117.041
UNCERTAINTY		0.42	0.42		0.418	0.460	0.081
400	20.225	101.03	80.80	83.01	-744.120	-641.858	83.818
500	33.286	120.09	86.80	87.76	-742.708	-616.453	64.401
600	42.707	136.46	93.75	91.82	-741.081	-591.348	51.482
700	50.010	150.91	100.90	95.86	-739.241	-566.537	42.276
800	56.001	163.98	107.98	100.05	-737.156	-542.000	35.389
900	61.133	176.02	114.89	104.43	-734.797	-517.744	30.049
1000	65.694	187.26	121.57	109.01	-732.118	-493.768	25.792
1074	23.183	149.70	126.52	112.50	-778.892	-476.333	23.167
1074	68.724	195.24	126.52	126.95	-729.981	-476.333	23.167
1100	69.846	197.87	128.02	126.95	-729.105	-470.077	22.322
1200	73.708	207.97	134.26	126.95	-725.734	-446.668	19.443
1300	77.358	217.67	140.31	126.95	-721.984	-423.569	17.019
1400	80.850	227.02	146.17	126.95	-717.847	-400.761	14.953
1500	84.225	236.09	151.87	126.95	-713.303	-378.278	13.173

MELTING POINT	1074	K	BOILING POINT	K
ENTHALPY OF MELTING	48.911	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>		kJ	MOLAR VOLUME	3.0560 J/bar 30.560 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MOLYBDENUM. M. P. 2890 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 5.3302 + 6.3165 \times 10^{-2} T + 1.3599 \times 10^{-3} T^2 - 2.4928 \times 10^{-6} T^3$$

(EQUATION VALID FROM 298 - 1074 K)

REFERENCE	247	247	247	COMPILED
	140		159	6- 8-76

## NITROGEN DIOXIDE

FORMULA WEIGHT 46.005

NO<sub>2</sub>: Ideal gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>p</sub> <sup>o</sup> J/mol·K			
298.15	0.000	240.06	240.06	36.97	33.095	51.251	-8.979
UNCERTAINTY		0.08	0.08		0.418	0.460	0.081
400	9.825	251.37	241.54	40.23	32.520	57.551	-7.515
500	16.214	260.68	244.47	43.30	32.165	63.853	-6.671
600	20.948	268.81	247.86	45.86	31.969	70.209	-6.112
700	24.661	276.04	251.38	47.94	31.882	76.591	-5.715
800	27.680	282.56	254.88	49.63	31.874	82.973	-5.418
900	30.200	288.48	258.28	51.00	31.923	89.378	-5.187
1000	32.334	293.92	261.59	52.12	32.003	95.743	-5.001
1100	34.175	298.93	264.75	53.03	32.110	102.114	-4.849
1200	35.779	303.57	267.79	53.78	32.230	108.483	-4.722
1300	37.188	307.90	270.71	54.39	32.356	114.828	-4.614
1400	38.436	311.95	273.51	54.88	32.485	121.167	-4.521
1500	39.544	315.75	276.21	55.27	32.605	127.495	-4.440
1600	40.537	319.33	278.79	55.58	32.719	133.815	-4.369
1700	41.429	322.71	281.28	55.82	32.824	140.120	-4.305
1800	42.234	325.90	283.67	56.00	32.916	146.442	-4.250

MELTING POINT	261.90 K	BOILING POINT	294.25 K
ENTHALPY OF MELTING	14.652 kJ	ENTHALPY OF VAPORIZATION	38.116 kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	10.196 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_p^o = 91.607 - 5.4423 \times 10^{-3} T - 1.1081 \times 10^{-5} T^2 + 9.9225 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	247	247	COMPILED 5-24-76
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DISODIUM MONOXIDE

FORMULA WEIGHT 61.979

Na<sub>2</sub>O: Crystals 298.15 to melting point 1193 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	75.27	75.27	69.10	-414.820	-376.089	65.889
UNCERTAINTY		0.84	0.84		0.280	0.290	0.051
400	18.575	96.65	78.08	76.30	-420.252	-362.418	47.327
500	30.644	114.25	83.61	81.34	-420.096	-347.976	36.353
600	39.433	129.44	90.01	85.26	-419.372	-333.611	29.044
700	46.216	142.83	96.61	88.47	-418.210	-319.391	23.833
800	51.672	154.82	103.15	91.20	-416.707	-305.375	19.939
900	56.200	165.71	109.51	93.60	-414.941	-291.569	16.922
1000	60.049	175.68	115.63	95.74	-412.974	-277.964	14.519

MELTING POINT	1193	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.5880 J/bar 25.880 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.1397 \times 10^2 + 7.4857 \times 10^{-3} T - 8.1335 \times 10^2 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	247	247	183	COMPILED
	63		265	6- 9-76

## SODIUM HYDROXIDE

FORMULA WEIGHT 39.997

NaOH: Crystals 298.15 to melting point 596 K. Liquid 596 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K			
298.15	0.000	64.43	64.43	59.53	-425.800	-379.651	66.514
UNCERTAINTY		0.84	0.84		0.085	0.125	0.022
400	15.877	82.72	66.85	64.94	-428.117	-363.727	47.498
500	26.576	98.16	71.58	75.16	-427.276	-347.707	36.325
596	45.686	123.36	77.67	84.97	-419.155	-332.978	29.183
596	56.778	134.45	77.67	86.10	-412.544	-332.978	29.183
600	56.972	134.98	78.01	86.08	-412.443	-332.421	28.940
700	61.086	148.21	87.12	85.48	-409.911	-319.286	23.826
800	64.099	159.58	95.48	84.88	-407.443	-306.507	20.013
900	66.378	169.54	103.16	84.29	-405.057	-294.024	17.065
1000	68.141	178.40	110.26	83.71	-402.774	-281.824	14.721
1100	69.531	186.35	116.82	83.12	-400.613	-269.823	12.813
1200	70.640	193.56	122.92	82.54	-495.983	-255.972	11.142
1300	71.534	200.14	128.61	81.97	-493.187	-236.090	9.486
1400	72.257	206.20	133.94	81.39	-490.491	-216.430	8.075
1500	72.846	211.79	138.94	80.82	-487.887	-196.934	6.858
1600	73.324	216.99	143.67	80.25	-485.377	-177.626	5.799
1700	73.712	221.83	148.12	79.68	-482.958	-158.462	4.869
1800	74.027	226.37	152.34	79.11	-480.628	-139.454	4.047

MELTING POINT	596 K	BOILING POINT	K
ENTHALPY OF MELTING	6.611 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	10.489 kJ	MOLAR VOLUME	1.8780 J/bar 18.780 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 88.445 - 5.5178 \times 10^{-3} T + 25.993 T^{-0.5} - 4.3125 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 596 - 1800 K)

REFERENCE	32	32	215	COMPILED
			32	5-24-76



NIوبيUM MONOXIDE

FORMULA WEIGHT 108.906

Mo: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	46.02	46.02	41.11	-419.660	-391.945	68.667
UNCERTAINTY		8.40	8.40		12.550	12.550	2.199
400	10.875	58.55	47.67	44.02	-419.377	-382.515	49.952
500	17.694	68.58	50.89	45.82	-418.979	-373.349	39.004
600	22.500	77.06	54.56	47.20	-418.520	-364.259	31.712
700	26.114	84.42	58.31	48.38	-418.021	-355.259	26.510
800	28.966	90.96	61.99	49.46	-417.488	-346.332	22.613
900	31.300	96.84	65.54	50.48	-416.925	-337.464	19.586
1000	33.268	102.21	68.94	51.46	-416.330	-328.670	17.168
1100	34.966	107.16	72.19	52.42	-415.704	-319.927	15.192
1200	36.460	111.76	75.30	53.36	-415.048	-311.254	13.549
1300	37.795	116.07	78.27	54.29	-414.359	-302.624	12.160
1400	39.007	120.13	81.12	55.21	-413.636	-294.062	10.972
1500	40.117	123.97	83.85	56.12	-412.881	-285.561	9.944
1600	41.145	127.62	86.48	57.02	-412.090	-277.090	9.046
1700	42.105	131.10	88.99	57.93	-411.264	-268.677	8.255
1800	43.009	134.44	91.43	58.83	-410.401	-260.317	7.554

MELTING POINT	2210	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	1.4970 J/bar 14.970 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

NIوبيUM.... M. P. 2740 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 43.088 + 8.8405 \times 10^{-3} T - 2.0913 T^{-0.5} - 3.9934 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	33	33	33	COMPILED 5-19-76
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## NIOBIUM DIOXIDE

FORMULA WEIGHT 124.905

NbO<sub>2</sub>: Alpha crystals 298.15 to 1150 K. Beta crystals 1150 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	54.51	54.51	57.45	-794.960	-739.194	129.504
UNCERTAINTY		0.30	0.30		8.370	8.370	1.466
400	15.375	72.22	56.85	63.14	-794.389	-720.221	94.052
500	25.410	86.82	61.41	67.83	-793.465	-701.780	73.315
600	32.835	99.57	66.73	72.03	-792.245	-683.549	59.508
700	38.717	110.97	72.25	75.93	-790.753	-665.558	49.665
800	43.600	121.35	77.75	79.62	-789.001	-647.785	42.296
900	47.800	130.93	83.13	83.15	-786.994	-630.241	36.578
1000	51.507	139.87	88.36	86.58	-784.738	-612.948	32.017
1100	54.848	148.28	93.43	89.92	-782.234	-595.883	28.296
1150	56.401	152.55	96.15	91.57	-780.870	-587.655	26.692
1150	60.059	156.20	96.15	83.05	-776.664	-587.655	26.692
1200	61.017	159.53	98.51	83.05	-775.755	-579.279	25.215
1300	62.712	166.18	103.47	83.05	-773.937	-562.973	22.621
1400	64.164	172.33	108.17	83.05	-772.195	-546.809	20.402
1500	65.424	178.06	112.64	83.05	-770.524	-530.779	18.483
1600	66.526	183.42	116.89	83.05	-768.924	-514.844	16.808
1700	67.498	188.46	120.96	83.05	-767.390	-499.028	15.333
1800	68.362	193.21	124.85	83.05	-765.921	-483.285	14.025

MELTING POINT	2175	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	4.5020 J/bar 45.020 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

NIOBIUM.... M. P. 2740 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 69.650 + 2.8178 \times 10^{-2} T - 3.5572 \times 10^{-5} T^{-0.5}$$

(EQUATION VALID FROM 298 - 1150 K)

REFERENCE	130	33	33	COMPILED
	189			8-11-76

DINIOBIUM PENTOXIDE

FORMULA WEIGHT 265.810

Nb<sub>2</sub>O<sub>5</sub>: Crystals 298.15 to melting point 1785 K. Liquid 1785 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	S <sub>T</sub> <sup>0</sup>	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	C <sub>P</sub> <sup>0</sup>	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	137.32	137.32	131.99	-1899.536	-1765.859	309.372
UNCERTAINTY		1.26	1.26		4.184	4.200	0.736
400	35.700	178.42	142.72	146.63	-1897.926	-1720.408	224.663
500	58.748	212.07	153.32	154.63	-1895.626	-1676.296	175.122
600	75.208	240.77	165.56	160.10	-1893.009	-1632.654	142.136
700	87.649	265.78	178.13	164.32	-1890.225	-1589.505	118.611
800	97.456	287.95	190.49	167.82	-1887.332	-1546.728	100.991
900	105.444	307.90	202.46	170.90	-1884.363	-1504.320	87.309
1000	112.137	326.05	213.91	173.70	-1881.316	-1462.256	76.381
1100	117.853	342.73	224.88	176.30	-1878.212	-1420.491	67.454
1200	122.827	358.18	235.35	178.76	-1875.048	-1379.034	60.028
1300	127.222	372.58	245.36	181.13	-1871.820	-1337.806	53.754
1400	131.157	386.09	254.93	183.41	-1868.525	-1296.863	48.387
1500	134.712	398.82	264.11	185.63	-1865.172	-1256.172	43.744
1600	137.963	410.87	272.91	187.80	-1861.747	-1215.675	39.688
1700	140.958	422.32	281.36	189.94	-1858.252	-1175.422	36.116
1785	173.186	485.63	312.44	191.73	-1836.357	-991.481	29.014
1785	231.598	544.04	312.44	242.25	-1732.092	-991.481	29.014
1800	201.181	490.99	289.81	242.25	-1751.288	-1135.904	32.963

MELTING POINT	1785	K	BOILING POINT	K
ENTHALPY OF MELTING	104.265	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	22.288	kJ	MOLAR VOLUME	9.3420 J/bar 93.420 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

NIOBIUM.... M. P. 2740 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.6605 \times 10^2 + 1.8368 \times 10^{-2} T - 2.7253 \times 10^{-5} T^2 - 2.1029 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1785 K)

REFERENCE	189	33	33	COMPILED 6- 2-76
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## NEODYMIUM SESQUIOXIDE (HEXAGONAL)

FORMULA WEIGHT 336.478

Nd<sub>2</sub>O<sub>3</sub>: Alpha crystals 298.15 to 1395 K. Beta crystals 1395 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	158.57	158.57	111.25	-1807.910	-1721.048	301.522
UNCERTAINTY		4.20	4.20		1.000	1.020	0.179
400	29.575	192.64	163.06	120.22	-1806.334	-1691.604	220.902
500	48.304	220.11	171.81	125.88	-1804.506	-1663.136	173.747
600	61.612	243.47	181.86	130.31	-1802.667	-1635.030	142.343
700	71.706	263.85	192.14	134.16	-1800.936	-1607.239	119.934
800	79.736	282.00	202.26	137.71	-1799.393	-1579.669	103.142
900	86.367	298.41	212.04	141.07	-1798.097	-1552.271	90.092
1000	92.000	313.44	221.44	144.33	-1797.103	-1525.013	79.659
1100	96.903	327.35	230.45	147.51	-1796.467	-1497.850	71.127
1200	101.251	340.32	239.07	150.65	-1801.924	-1470.322	64.002
1300	105.170	352.50	247.33	153.75	-1815.300	-1455.616	58.488
1395	108.373	363.26	254.89	156.70	-1815.283	-1415.402	52.999
1395	109.043	363.93	254.89	155.64	-1814.348	-1415.402	52.999
1400	109.200	364.47	255.27	155.64	-1814.331	-1413.973	52.756
1500	112.299	375.21	262.91	155.64	-1813.995	-1385.400	48.244
1600	115.008	385.25	270.24	155.64	-1813.702	-1356.830	44.296
1700	117.399	394.69	277.29	155.64	-1813.445	-1328.291	40.814
1800	119.523	403.58	284.06	155.64	-1813.220	-1299.734	37.717

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	21.004 kJ	MOLAR VOLUME	4.5920 J/bar 45.920 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

NEODYMIUM.. ALPHA-BETA 1128, M. P. 1289 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 1.1574 \times 10^2 + 2.9779 \times 10^{-2} T - 1.1883 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1395 K)

REFERENCE	210	235	235	COMPILED
				8-11-76

BUNSENITE

FORMULA WEIGHT 74.699

Min: Crystals 298.15 to melting point 2257 K.  $\alpha$ - $\beta$  transition at 525 K and  $\beta$ - $\gamma$  transition at 565 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K			
298.15	0.000	37.99	37.99	48.04	-239.743	-211.581	37.068
UNCERTAINTY		0.17	0.17		0.418	0.460	0.081
400	12.175	52.01	39.83	52.74	-239.170	-202.044	26.384
500	21.212	64.73	43.52	53.22	-237.923	-192.873	20.149
600	27.747	75.79	48.04	50.94	-236.734	-184.009	16.019
700	31.130	83.71	52.58	51.91	-236.535	-175.222	13.075
800	33.786	90.71	56.92	52.87	-236.052	-166.504	10.872
900	35.956	96.99	61.03	53.83	-235.562	-157.838	9.161
1000	37.795	102.71	64.91	54.79	-235.099	-149.219	7.794
1100	39.384	107.98	68.60	55.75	-234.680	-140.663	6.680
1200	40.787	112.87	72.08	56.71	-234.284	-132.122	5.751
1300	42.050	117.45	75.40	57.67	-233.886	-123.633	4.968
1400	43.200	121.76	78.56	58.64	-233.466	-115.166	4.297
1500	44.261	125.84	81.58	59.60	-232.995	-106.740	3.717
1600	45.250	129.71	84.46	60.56	-232.454	-98.334	3.210
1700	46.179	133.41	87.23	61.52	-231.826	-89.970	2.764
1800	47.058	136.96	89.90	62.48	-249.077	-80.885	2.347

MELTING POINT	2257	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	6.694	kJ	MOLAR VOLUME	1.0970 J/bar 10.970 $\text{cm}^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

NICKEL..... CURIE P. 631, M. P. 1726 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 45.175 + 9.6149 \times 10^{-3} T$$

(EQUATION VALID FROM 565 - 1800 K)

REFERENCE	129	120	23	COMPILED
			263	6-21-76

## PHOSPHORUS MONOXIDE

FORMULA WEIGHT 46.973

PO: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	222.77	222.77	31.76	-12.134	-41.157	7.211
UNCERTAINTY		0.02	0.02		4.184	4.200	0.736
400	8.150	232.18	224.03	32.39	-12.654	-51.000	6.660
500	13.086	239.49	226.40	33.23	-13.292	-60.510	6.322
600	16.507	245.62	229.11	33.99	-14.027	-69.890	6.084
700	19.051	250.91	231.86	34.63	-14.871	-79.139	5.905
800	21.032	255.57	234.54	35.16	-101.258	-110.430	7.210
900	22.622	259.74	237.12	35.59	-101.248	-111.578	6.476
1000	23.942	263.51	239.57	35.95	-101.231	-112.726	5.888
1100	25.048	266.95	241.90	36.25	-101.218	-113.877	5.408
1200	25.992	270.11	244.12	36.49	-101.210	-115.025	5.007
1300	26.807	273.04	246.23	36.68	-101.201	-116.174	4.668
1400	27.521	275.76	248.24	36.84	-101.193	-117.317	4.377
1500	28.144	278.31	250.17	36.97	-101.198	-118.475	4.126
1600	28.699	280.70	252.00	37.07	-101.205	-119.633	3.906
1700	29.194	282.95	253.76	37.14	-101.218	-120.785	3.711
1800	29.637	285.07	255.43	37.20	-101.236	-121.925	3.530

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
$H_{298}^0 - H_0^0$	9.393 kJ	MOLAR VOLUME	J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

PHOSPHORUS. SUBLINES 704 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 49.471 - 1.9035 \times 10^{-3} T - 3.8115 \times 10^2 T^{-0.5} + 4.3831 \times 10^5 T^{-2}$$

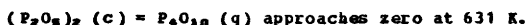
(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	32	32	32	COMPILED 5-24-76
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PHOSPHORUS PENTOXIDE

FORMULA WEIGHT 141.945

P<sub>2</sub>O<sub>5</sub>: Crystals 298.15 to 1000 K. The free energy change for the reaction



TEMP. K	(H <sub>T</sub> <sup>o</sup> - H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> - H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>P</sub> <sup>o</sup> J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	115.50	115.50	105.86	-1470.000	-1337.897	234.396
UNCERTAINTY		0.40	0.40		4.200	4.200	0.736
400	31.327	151.46	120.13	125.42	-1469.571	-1292.781	168.820
500	54.936	184.69	129.75	148.01	-1467.072	-1248.837	130.466
600	74.720	216.28	141.56	170.60	-1462.646	-1205.572	104.955
700	92.180	246.59	154.41	153.97	-1456.387	-1163.209	86.800
800	108.089	275.86	167.77	153.97	-1619.194	-1166.197	76.146
900	122.861	304.23	181.37	153.97	-1607.236	-1110.251	64.438
1000	136.758	331.80	195.04	153.97	-1593.367	-1055.763	55.147

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	kJ	MOLAR VOLUME	5.9400 J/bar 59.400 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

PHOSPHORUS. SUBLINES 704 K.

HEAT CAPACITY EQUATION

C<sub>P</sub><sup>o</sup> = 35.041 + 0.22594 T  
(EQUATION VALID FROM 298 - 631 K)

REFERENCE	247	215	215	COMPILED 03-15-79
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## PHOSPHORUS PENTOXIDE (DIMERIC)

FORMULA WEIGHT 283.889

(P<sub>2</sub>O<sub>5</sub>)<sub>2</sub>: Crystals 289.15 to 1000 K. The free energy change for the reaction(P<sub>2</sub>O<sub>5</sub>)<sub>2</sub> (c) = P<sub>4</sub>O<sub>10</sub> (g) approaches zero at 631 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	231.00	231.00	211.71	-2940.000	-2675.794	468.791
UNCERTAINTY		0.80	0.80		8.400	8.400	1.472
400	62.665	302.92	240.26	250.84	-2939.138	-2585.558	337.641
500	109.880	369.37	259.49	296.03	-2934.140	-2497.670	260.931
600	149.445	432.56	283.11	341.22	-2925.289	-2411.141	209.909
700	184.364	493.19	308.83	307.94	-2912.772	-2326.417	173.600
800	216.176	551.72	335.54	307.94	-3238.390	-2332.395	152.290
900	245.721	608.46	362.73	307.94	-3214.473	-2220.501	128.876
1000	273.516	663.59	390.08	307.94	-3186.734	-2111.526	110.296

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	34.551 kJ	MOLAR VOLUME	11.8800 J/bar 118.800 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

## HEAT CAPACITY EQUATION

$$C_P^0 = 70.082 + 0.45190 T$$

(EQUATION VALID FROM 298 - 631 K)

REFERENCE	247	215	215	COMPILED 03-15-79
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ORTHOPHOSPHORIC ACID (CRYSTAL)

FORMULA WEIGHT 97.995

H<sub>3</sub>PO<sub>4</sub>: Crystals 298.15 to melting point 315.5 K. Above 315.5 K the data tabulated are a metastable extrapolation.

TEMP. K	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	110.54	110.54	106.06	-1266.920	-1112.290	194.869
UNCERTAINTY		0.42	0.42		2.090	2.510	0.440
400	30.925	146.02	115.09	136.91	-1267.310	-1059.332	138.335
500	55.156	179.82	124.66	167.20	-1265.005	-1007.551	105.259
600	76.353	212.98	136.63	197.48	-1260.004	-956.478	83.269
700	95.821	245.70	149.88	227.77	-1252.301	-906.476	67.642
800	114.209	278.09	163.88	258.06	-1327.312	-879.923	57.453
900	131.878	310.24	178.36	288.35	-1313.073	-824.804	47.871
1000	149.037	342.18	193.14	318.64	-1295.984	-771.449	40.297

MELTING POINT	315.50 K	BOILING POINT	K
ENTHALPY OF MELTING	13.400 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	4.8520 J/bar 48.520 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			
PHOSPHORUS. SUBLIMES 704 K.			

HEAT CAPACITY EQUATION

$$C_P^0 = 15.756 + 0.30288 T$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	32	32	32	COMPILED 5-19-76
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## ORTHOPHOSPHORIC ACID (LIQUID)

FORMULA WEIGHT 97.995

 $H_3PO_4$ : Liquid 298.15 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	150.78	150.78	145.05	-1254.200	-1111.700	194.766
UNCERTAINTY		4.20	4.20		2.090	2.510	0.440
400	40.850	197.69	156.84	175.73	-1250.620	-1063.310	138.855
500	70.830	240.14	169.31	205.85	-1244.448	-1017.154	106.262
600	95.843	280.34	184.50	235.98	-1235.590	-972.480	84.662
700	118.014	318.97	200.96	266.10	-1224.046	-929.510	69.361
800	138.407	356.47	218.06	296.22	-1295.233	-910.548	59.453
900	157.611	393.10	235.49	326.35	-1277.193	-863.498	50.116
1000	175.995	429.04	253.04	356.47	-1256.306	-818.631	42.761

MELTING POINT	315.50 K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

PHOSPHORUS. SUBLIMES 704 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 55.239 + 0.30123 T$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	32	32	32	COMPILED 5-19-76
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LITHARGE (RED)

FORMULA WEIGHT 223.199

PbO: Tetragonal crystals 298.15 to 1400 K. Massicot (orthorhombic) is the stable phase above 762 K. See table for lead monoxide (reference state).

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	66.32	66.32	45.77	-219.409	-189.202	33.148
UNCERTAINTY		0.84	0.84		0.830	0.900	0.158
400	12.325	80.51	68.18	50.51	-218.740	-178.974	23.372
500	20.250	92.09	71.84	53.20	-217.863	-169.133	17.669
600	25.910	101.97	76.06	55.13	-216.909	-159.474	13.883
700	30.199	110.59	80.39	56.70	-220.786	-149.183	11.132
800	33.599	118.25	84.65	58.08	-219.733	-139.025	9.077
900	36.389	125.17	88.78	59.35	-218.547	-129.006	7.487
1000	38.747	131.48	92.73	60.55	-217.229	-119.119	6.222
1100	40.782	137.31	96.53	61.71	-215.791	-109.388	5.194
1200	42.572	142.73	100.16	62.83	-214.236	-99.786	4.344
1300	44.174	147.80	103.63	63.93	-212.568	-90.303	3.628
1400	45.621	152.58	106.96	65.02	-210.800	-80.978	3.021

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.3910 J/bar 23.910 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LEAD..... M. P. 600.6, B. P. 2021 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 51.017 + 1.0272 \times 10^{-2} T - 7.3872 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	32	32	32	COMPILED 6- 7-76
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## MASSICOT (YELLOW)

FORMULA WEIGHT 223.199

PbO: Orthorhombic crystals 298.15 to 1170 K. See table for lead monoxide  
(reference state). Liquid 1170 to 1789 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	68.70	68.70	45.77	-218.070	-188.573	33.037
UNCERTAINTY		0.21	0.21		0.630	0.700	0.123
400	12.025	82.57	70.54	48.53	-217.521	-178.579	23.320
500	19.532	93.61	74.08	50.46	-216.883	-168.913	17.646
600	24.827	102.96	78.13	52.10	-216.220	-159.379	13.875
700	28.831	111.10	82.27	53.60	-220.404	-149.158	11.130
800	32.017	118.36	86.34	55.03	-219.659	-139.039	9.078
900	34.656	124.92	90.26	56.41	-218.768	-129.002	7.487
1000	36.894	130.93	94.04	57.76	-217.743	-119.083	6.220
1100	38.852	136.50	97.65	59.10	-216.575	-109.281	5.189
1170	38.255	118.42	100.16	60.03	-241.224	-102.532	4.578
1170	40.069	140.23	100.16	65.00	-215.702	-102.532	4.578
1200	40.679	141.78	101.10	65.00	-215.271	-99.582	4.335
1300	42.510	146.94	104.43	65.00	-213.434	-90.007	3.617
1400	44.099	151.74	107.64	65.00	-211.610	-80.590	3.007
1500	45.490	156.22	110.73	65.00	-209.794	-71.303	2.483
1600	46.725	160.43	113.70	65.00	-208.003	-62.126	2.028
1700	47.831	164.40	116.57	65.00	-206.229	-53.068	1.631

MELTING POINT	1170	K	BOILING POINT	1789	K
ENTHALPY OF MELTING	25.522	kJ	ENTHALPY OF VAPORIZATION	207.233	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.3150	J/bar 23.150 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

LEAD..... M. P. 600.6, B. P. 2021 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 45.188 + 1.2863 \times 10^{-2} T - 2.8918 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1170 K)

REFERENCE 32 32 32 COMPILED

6-7-76

LEAD MONOXIDE (REFERENCE)

FORMULA WEIGHT 223.199

PbO: Litharge (red) 298.15 to 762 K. Massicot (yellow) 762 to 1170 K.

Liquid 1170 to 1789 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	66.32	66.32	45.77	-219.409	-189.202	33.148
UNCERTAINTY		0.84	0.84		0.830	0.900	0.158
400	12.325	80.51	68.18	50.51	-218.740	-178.974	23.372
500	20.250	92.09	71.84	53.20	-217.863	-169.133	17.669
600	25.910	101.97	76.06	55.13	-216.909	-159.474	13.884
700	30.199	110.59	80.39	56.70	-220.786	-149.183	11.132
762	32.385	114.64	82.24	57.57	-220.066	-141.863	9.725
762	32.824	115.06	82.24	54.50	-219.731	-141.863	9.725
800	33.859	118.37	84.51	55.03	-219.525	-138.913	9.070
900	36.257	124.90	88.64	56.41	-218.666	-128.878	7.480
1000	38.305	130.88	92.57	57.76	-217.671	-118.956	6.214
1100	40.090	136.40	96.31	59.10	-216.552	-109.146	5.183
1170	41.214	139.86	98.64	60.04	-215.702	-102.093	4.558
1170	63.027	161.67	98.64	65.00	-190.180	-102.093	4.558
1200	63.063	163.22	100.16	65.00	-189.647	-99.785	4.344
1300	63.172	168.38	105.21	65.00	-187.871	-92.360	3.711
1400	63.286	173.18	109.89	65.00	-186.070	-85.088	3.175
1500	63.398	177.66	114.26	65.00	-184.255	-77.935	2.714
1600	63.514	181.87	118.36	65.00	-182.420	-70.908	2.315
1700	63.632	185.84	122.21	65.00	-180.571	-63.994	1.966

MELTING POINT	1170	K	BOILING POINT	1789	K
ENTHALPY OF MELTING	25.522	kJ	ENTHALPY OF VAPORIZATION	207.233	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.3910	J/bar
				23.910	cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LEAD..... M. P. 600.6, B. P. 2021 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = 51.017 + 1.0272 \times 10^{-2} T - 7.3872 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 762 K)

REFERENCE	32	32	32	COMPILED
	115			6-29-76

## PLATTNERITE

FORMULA WEIGHT 239.199

PbO<sub>2</sub>: Crystals 298.15 to 1200 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	71.80	71.80	61.17	-274.470	-215.314	37.722
UNCERTAINTY		0.42	0.42		2.929	3.000	0.526
400	16.600	90.90	74.30	68.23	-273.603	-195.219	25.493
500	27.310	106.54	79.23	71.82	-272.438	-175.758	18.361
600	34.930	119.85	84.92	74.11	-271.184	-156.536	13.628
700	40.653	131.41	90.76	75.79	-274.783	-136.736	10.203
800	45.131	141.62	96.49	77.14	-273.488	-117.104	7.646
900	48.756	150.77	102.01	78.30	-272.097	-97.623	5.666
1000	51.760	159.08	107.32	79.34	-270.624	-78.324	4.091
1100	54.313	166.69	112.38	80.31	-269.068	-59.177	2.810
1200	56.517	173.71	117.19	81.22	-267.438	-40.158	1.748

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	10.966 kJ	MOLAR VOLUME	2.5010 J/bar 25.010 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LEAD..... M. P. 600.6, B. P. 2021 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 73.119 + 7.4840 \times 10^{-3} T - 1.2605 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	32	32	32	COMPILED 6-7-76
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MINIUM

FORMULA WEIGHT 685.598

Pb<sub>3</sub>O<sub>4</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	211.96	211.96	154.93	-718.686	-601.358	105.356
UNCERTAINTY		6.69	6.69		6.276	6.300	1.104
400	42.025	260.32	218.29	172.95	-716.171	-561.615	73.340
500	69.264	300.06	230.80	182.86	-712.835	-523.365	54.676
600	88.798	334.04	245.24	189.76	-709.171	-485.803	42.293
700	103.624	363.71	260.09	195.24	-719.952	-446.483	33.317
800	115.377	390.10	274.72	199.97	-715.914	-407.698	26.620
900	125.022	413.90	288.88	204.25	-711.449	-369.404	21.440
1000	133.143	435.63	302.49	208.26	-706.591	-331.661	17.324
1100	140.147	455.66	315.51	212.10	-701.350	-294.438	13.982
1200	146.298	474.28	327.98	215.81	-695.745	-257.697	11.217
1300	151.785	491.69	339.90	219.44	-689.790	-221.400	8.896
1400	156.743	508.09	351.35	223.00	-683.508	-185.640	6.926
1500	161.280	523.59	362.31	226.52	-676.899	-150.294	5.234
1600	165.466	538.32	372.85	230.00	-669.986	-115.426	3.768
1700	169.364	552.36	383.00	233.46	-662.772	-80.981	2.488
1800	173.020	565.80	392.78	236.89	-655.270	-46.924	1.362

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	30.188 kJ	MOLAR VOLUME	7.6810 J/bar 76.810 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LEAD..... M. P. 600.6, B. P. 2021 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.7793 \times 10^2 + 3.3260 \times 10^{-2} T - 2.9259 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	32	32	32	COMPILED 6-7-76
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## PRASEODYMIUM SESQUIOXIDE (HEX)

FORMULA WEIGHT 329.814

Pr<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
					kJ/mol	kJ/mol	
298.15	0.000	158.57	158.57	120.40	-1809.580	-1721.025	301.518
UNCERTAINTY		4.20	4.20		6.690	6.700	1.174
400	31.025	194.79	163.76	126.08	-1807.380	-1691.286	220.860
500	50.492	223.40	172.91	130.46	-1804.946	-1662.541	173.685
600	64.138	247.53	183.39	134.20	-1802.579	-1634.282	142.278
700	74.391	268.47	194.08	137.57	-1800.364	-1606.415	119.873
800	82.484	287.04	204.56	140.68	-1798.355	-1578.839	103.088
900	89.111	303.78	214.67	143.61	-1796.589	-1551.510	90.048
1000	94.703	319.06	224.36	146.40	-1795.082	-1524.352	79.624
1100	99.526	333.14	233.61	149.10	-1799.927	-1497.163	71.095
1200	103.767	346.23	242.46	151.72	-1797.911	-1469.729	63.976
1300	107.553	358.47	250.92	154.27	-1810.328	-1441.323	57.913
1400	110.979	370.00	259.02	156.77	-1808.803	-1413.023	52.721
1500	114.114	380.89	266.78	159.23	-1807.071	-1384.806	48.223
1600	117.009	391.25	274.24	161.65	-1805.136	-1356.712	44.292
1700	119.425	401.12	281.69	164.05	-1803.472	-1329.249	40.843
1800	122.235	410.56	288.32	166.41	-1800.649	-1300.915	37.752

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.6530 J/bar 46.530 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

PRASEODYMIUM ALPHA-BETA 1068, M. P. 1204 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.3845 \times 10^2 + 2.0864 \times 10^{-2} T - 4.0616 \times 10^2 T^{-0.5} - 6.5701 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	200	281	235	COMPILED 6-14-76
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PRASEODYMIUM OXIDE

FORMULA WEIGHT 170.235

PrO<sub>1.833</sub>: Alpha crystals 298.15 to 760 K. Beta crystals 760 to 1100 K.

TEMP. K	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>P</sub> <sup>o</sup> J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	79.91	79.91	65.86	-1904.560	-1796.610	314.760
UNCERTAINTY		4.20	4.20		6.690	6.700	1.174
400	17.400	99.95	82.55	70.74	-1903.208	-1831.940	239.228
500	28.542	116.25	87.71	75.54	-1901.609	-1814.308	189.540
600	36.773	130.44	93.67	80.33	-1899.777	-1797.010	156.444
700	43.337	143.19	99.85	85.12	-1897.736	-1780.051	132.830
760	46.446	150.72	104.28	87.99	-1896.563	-1770.536	121.689
760	48.553	152.83	104.28	87.18	-1894.962	-1770.536	121.689
800	50.707	157.15	106.44	89.16	-1894.012	-1763.732	115.160
900	55.256	167.94	112.68	94.13	-1891.638	-1747.588	101.428
1000	59.393	178.11	118.72	99.10	-1889.048	-1731.707	90.455
1100	63.229	187.79	124.56	104.07	-1889.283	-1716.020	81.487

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	kJ	MOLAR VOLUME	2.4600 J/bar 24.600 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

PRASEODYMIUM ALPHA-BETA 1068, M. P. 1204 K.

HEAT CAPACITY EQUATIONS

$$C_P^o = 51.577 + 4.7918 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 760 K)

$$C_P^o = 49.403 + 4.9701 \times 10^{-2} T$$

(EQUATION VALID FROM 760 - 1100 K)

REFERENCE	200	281	281	COMPILED 5-18-76
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## SULFUR DIOXIDE

FORMULA WEIGHT 64.059

SO<sub>2</sub>: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	248.22	248.22	39.87	-296.810	-300.170	52.589
UNCERTAINTY		0.06	0.06		0.200	0.251	0.044
400	10.650	260.48	249.83	43.66	-300.222	-300.831	39.285
500	17.562	270.56	253.00	46.65	-302.690	-300.649	31.409
600	22.613	279.28	256.67	48.99	-304.665	-300.095	26.126
700	26.519	286.98	260.46	50.84	-306.256	-299.190	22.326
800	29.654	293.86	264.21	52.30	-362.267	-303.629	19.825
900	32.233	300.10	267.87	53.48	-362.212	-296.262	17.195
1000	34.412	305.78	271.37	54.44	-362.111	-288.927	15.092
1100	36.268	311.01	274.74	55.21	-361.988	-281.628	13.373
1200	37.875	315.84	277.96	55.85	-361.840	-274.318	11.941
1300	39.278	320.33	281.05	56.36	-361.678	-267.027	10.729
1400	40.514	324.52	284.01	56.78	-361.510	-259.754	9.692
1500	41.610	328.45	286.84	57.12	-361.340	-252.497	8.793
1600	42.587	332.15	289.56	57.38	-361.166	-245.254	8.007
1700	43.464	335.63	292.17	57.59	-360.996	-238.012	7.313
1800	44.253	338.93	294.68	57.74	-360.834	-230.785	6.697

MELTING POINT	197.64 K	BOILING POINT	263.08 K
ENTHALPY OF MELTING	7.401 kJ	ENTHALPY OF VAPORIZATION	24.937 kJ
$H_{298}^0 - H_0^0$	10.548 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 86.219 - 4.3073 \times 10^{-3} T - 8.8646 \times 10^{-2} T^{-0.5} + 5.5769 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	35	35	COMPILED 5-24-76
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SULFUR TRIOXIDE

FORMULA WEIGHT 80.058

SO<sub>3</sub>: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS		
					ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	256.76	256.76	50.66	-395.722	-371.046	65.006
UNCERTAINTY		0.84	0.84		0.711	0.795	0.139
400	13.875	272.72	258.84	57.94	-399.356	-362.087	47.284
500	23.240	286.24	263.00	63.21	-401.807	-352.431	36.818
600	30.245	298.13	267.88	67.16	-403.624	-342.423	29.811
700	35.746	308.72	272.97	70.19	-404.962	-332.097	24.781
800	40.205	318.26	278.05	72.55	-460.657	-327.167	21.362
900	43.911	326.91	283.00	74.42	-460.233	-310.440	18.018
1000	47.034	334.83	287.80	75.90	-459.748	-293.824	15.348
1100	49.715	342.13	292.42	77.08	-459.209	-277.274	13.167
1200	52.036	348.88	296.84	78.03	-458.634	-260.755	11.350
1300	54.065	355.15	301.09	78.78	-458.035	-244.279	9.815
1400	55.850	361.01	305.16	79.36	-457.431	-227.870	8.502
1500	57.435	366.50	309.06	79.82	-456.818	-211.490	7.365
1600	58.845	371.67	312.82	80.16	-456.208	-195.168	6.372
1700	60.106	376.53	316.42	80.40	-455.608	-178.867	5.496
1800	61.238	381.13	319.89	80.56	-455.026	-162.600	4.719

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.2760 \times 10^2 - 7.8140 \times 10^{-3} T + 6.1238 \times 10^{-5} T^2 - 1.4073 \times 10^{-8} T^{-0.5}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	247	247	COMPILED 5-24-76
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## SCANDIUM SESQUIOXIDE

FORMULA WEIGHT 137.910

Sc<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	76.99	76.99	96.98	-1908.820	-1819.371	318.748
UNCERTAINTY		0.42	0.42		2.510	2.520	0.441
400	25.400	106.24	80.84	104.70	-1908.470	-1788.852	233.601
500	42.016	130.41	88.39	111.77	-1907.532	-1759.042	183.767
600	54.087	151.26	97.17	116.85	-1906.270	-1729.459	150.563
700	63.336	169.57	106.23	120.63	-1904.845	-1700.103	126.864
800	70.682	185.87	115.19	123.48	-1903.370	-1670.950	109.102
900	76.678	200.55	123.87	125.66	-1901.927	-1641.972	95.298
1000	81.661	213.88	132.22	127.34	-1900.590	-1613.180	84.264
1100	85.874	226.08	140.21	128.62	-1899.407	-1584.500	75.242
1200	89.478	237.31	147.83	129.60	-1898.429	-1555.896	67.727
1300	92.593	247.71	155.12	130.32	-1897.694	-1527.391	61.372
1400	95.307	257.39	162.08	130.83	-1897.241	-1498.927	55.926
1500	97.687	266.43	168.74	131.17	-1897.102	-1470.486	51.207
1600	99.786	274.90	175.11	131.36	-1897.305	-1442.048	47.078
1700	101.646	282.87	181.22	131.43	-1906.511	-1413.093	43.419
1800	103.299	290.38	187.08	131.39	-1907.787	-1384.040	40.164

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	13.975 kJ	MOLAR VOLUME	3.5910 J/bar 35.910 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SCANDIUM... ALPHA-BETA 1608, M. P. 1812 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.9455 \times 10^2 - 1.2212 \times 10^{-2} T - 1.7527 \times 10^3 T^{-0.5} + 4.2670 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	203	281	264	COMPILED
			162	6- 9-76

SILICON MONOXIDE

FORMULA WEIGHT 44.085

SiO: Ideal gas 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	211.57	211.57	29.90	-100.416	-127.305	22.304
UNCERTAINTY		0.84	0.84		8.368	8.500	1.489
400	7.775	220.54	212.76	31.22	-100.972	-136.410	17.813
500	12.590	227.64	215.05	32.40	-101.605	-145.200	15.169
600	15.975	233.63	217.65	33.37	-102.293	-153.848	13.394
700	18.519	238.84	220.32	34.15	-103.018	-162.385	12.117
800	20.514	243.44	222.93	34.78	-103.776	-170.813	11.153
900	22.122	247.57	225.45	35.28	-104.567	-179.150	10.398
1000	23.464	251.31	227.85	35.70	-105.374	-187.394	9.788
1100	24.592	254.73	230.14	36.03	-106.210	-195.563	9.287
1200	25.557	257.87	232.31	36.30	-107.069	-203.627	8.864
1300	26.392	260.79	234.40	36.52	-107.951	-211.653	8.504
1400	27.121	263.50	236.38	36.70	-108.858	-219.598	8.193
1500	27.765	266.04	238.27	36.84	-109.785	-227.474	7.921
1600	28.336	268.42	240.08	36.95	-110.734	-235.286	7.681
1700	28.845	270.66	241.81	37.03	-162.215	-242.600	7.454
1800	29.301	272.78	243.48	37.09	-162.923	-247.306	7.177

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	8.711 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 $cm^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 50.373 - 2.0840 \times 10^{-3} T - 4.0900 \times 10^{-5} T^{-0.5} + 3.4095 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	247	247	COMPILED 5-24-76
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QUARTZ FORMULA WEIGHT 60.085

SiO<sub>2</sub>: Alpha quartz 298.15 to 844 K. Beta quartz 844 to 1800 K.

Beta quartz is metastable above 1140 K.

TEMP.	FORMATION FROM THE ELEMENTS					GIBBS		Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	S <sub>T</sub> <sup>0</sup>	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	C <sub>p</sub> <sup>0</sup>	ENTHALPY	FREE ENERGY		
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	41.46	41.46	44.59	-910.700	-856.288	150.019	
UNCERTAINTY		0.20	0.20		1.000	1.100	0.193	
400	12.575	55.91	43.34	53.44	-910.848	-837.660	109.388	
500	21.376	68.51	47.13	59.47	-910.540	-819.395	85.602	
600	28.152	79.81	51.66	64.47	-909.897	-801.219	69.753	
700	33.667	90.09	56.42	68.99	-908.952	-783.176	58.442	
800	38.350	99.58	61.23	73.24	-907.711	-765.287	49.968	
844	40.059	103.76	63.69	75.06	-907.160	-757.697	46.894	
844	40.623	104.31	63.69	67.39	-906.684	-757.697	46.894	
900	42.356	108.35	65.99	67.96	-906.260	-747.572	43.388	
1000	44.967	115.56	70.59	68.96	-905.502	-729.982	38.131	
1100	47.194	122.18	74.99	69.96	-904.732	-712.474	33.833	
1200	49.132	128.31	79.18	70.97	-903.937	-695.017	30.253	
1300	50.851	134.03	83.18	71.97	-903.108	-677.649	27.228	
1400	52.393	139.40	87.01	72.97	-902.241	-660.349	24.638	
1500	53.800	144.47	90.67	73.97	-901.321	-643.096	22.395	
1600	55.092	149.28	94.19	74.98	-900.352	-625.920	20.434	
1700	56.291	153.85	97.56	75.98	-949.834	-608.355	18.693	
1800	57.413	158.22	100.81	76.98	-948.460	-588.298	17.072	

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	6.916 kJ	MOLAR VOLUME	2.2688 J/bar 22.688 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATIONS

$$C_p^0 = 44.603 + 3.7754 \times 10^{-2} T - 1.0018 \times 10^{-4} T^2$$

(EQUATION VALID FROM 298 - 844 K)

$$C_p^0 = 58.928 + 1.0031 \times 10^{-2} T$$

(EQUATION VALID FROM 844 - 1800 K)

REFERENCE	247	35	35	COMPILED
		278	284	7-16-76

CRISTOBALITE

FORMULA WEIGHT 60.085

SiO<sub>2</sub>: Alpha cristobalite 298.15 to 523 K. Beta cristobalite 523 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	43.40	43.40	44.18	-908.346	-854.512	149.708
UNCERTAINTY		0.13	0.13		2.090	2.130	0.373
460	12.625	57.93	45.30	50.73	-908.474	-836.094	109.183
500	21.482	70.56	49.08	68.59	-908.133	-818.613	85.458
523	22.936	73.77	50.84	77.54	-908.055	-813.854	81.284
523	25.504	76.34	50.84	58.33	-906.712	-813.854	81.284
600	29.955	84.60	54.64	62.06	-906.461	-800.657	69.704
700	34.784	94.42	59.64	65.23	-905.816	-783.071	58.434
800	38.730	103.28	64.55	67.34	-905.053	-765.589	49.988
900	41.989	111.30	69.31	68.82	-904.236	-748.203	43.425
1000	44.735	118.61	73.88	69.92	-903.380	-730.910	38.179
1100	47.065	125.32	78.26	70.77	-902.520	-713.716	33.892
1200	49.069	131.50	82.43	71.44	-901.659	-696.567	30.321
1300	50.812	137.24	86.43	72.00	-900.804	-679.518	27.303
1400	52.343	142.60	90.26	72.47	-899.957	-662.545	24.720
1500	53.698	147.61	93.91	72.87	-899.120	-645.605	22.482
1600	54.907	152.32	97.41	73.22	-898.293	-628.725	20.526
1700	55.994	156.77	100.78	73.53	-947.986	-611.471	18.788
1800	56.976	160.98	104.00	73.82	-946.892	-591.698	17.171

MELTING POINT	1996	K	BOILING POINT	K
ENTHALPY OF MELTING	8.159	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	7.040	kJ	MOLAR VOLUME	2.5739 J/bar 25.739 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = -4.1596 \times 10^3 + 2.5480 T + 7.1680 \times 10^4 T^{-0.5} - 6.2859 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 298 - 523 K)

$$C_P^0 = 72.753 + 1.3004 \times 10^{-3} T - 4.1320 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 523 - 1800 K)

REFERENCE	247	247	247	COMPILED
	172	278		6- 8-76

TRIDYMITTE FORMULA WEIGHT 60.085

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SiO<sub>2</sub>: Alpha tridymite 298.15 to 390 K. Beta tridymite 390 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	43.93	43.93	44.60	-907.488	-853.812	149.585
UNCERTAINTY		0.42	0.42		2.385	2.427	0.425
390	11.640	57.15	45.52	54.15	-907.593	-837.302	112.145
390	12.069	57.57	45.52	56.41	-907.426	-837.302	112.145
400	13.275	59.01	45.73	56.97	-907.356	-835.408	109.094
500	22.468	72.21	49.74	61.17	-906.782	-817.487	85.403
600	29.155	83.61	54.45	63.84	-906.083	-799.685	69.619
700	34.253	93.60	59.35	65.73	-905.330	-782.011	58.355
800	38.281	102.48	64.20	67.18	-904.554	-764.450	49.914
900	41.556	110.46	68.90	68.35	-903.768	-746.979	43.354
1000	44.290	117.72	73.43	69.35	-902.967	-729.607	38.111
1100	46.607	124.37	77.76	70.21	-902.165	-712.316	33.825
1200	48.607	130.51	81.90	70.98	-901.356	-695.076	30.256
1300	50.355	136.22	85.87	71.67	-900.541	-677.929	27.240
1400	51.900	141.56	89.66	72.32	-899.719	-660.851	24.657
1500	53.283	146.57	93.29	72.92	-898.885	-643.810	22.420
1600	54.527	151.29	96.76	73.49	-898.043	-626.827	20.464
1700	55.659	155.76	100.10	74.03	-947.697	-609.465	18.727
1800	56.694	160.01	103.32	74.54	-946.542	-589.602	17.110

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.6530 J/bar 26.530 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 74.904 + 3.0999 \times 10^{-3} T - 2.3669 \times 10^2 T^{-0.5} - 1.1740 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 390 - 1800 K)

REFERENCE	172	285	148	COMPILED 6-28-76
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COESITE FORMULA WEIGHT 60.085

SiO<sub>2</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
					kJ/mol	kJ/mol	
298.15	0.000	40.38	40.38	45.40	-905.584	-850.850	149.066
UNCERTAINTY		0.42	0.42		2.092	2.134	0.374
400	12.475	54.72	42.24	52.54	-905.772	-832.108	108.663
500	21.102	67.11	46.01	58.45	-905.561	-813.716	85.009
600	27.708	78.17	50.46	62.76	-905.047	-795.385	69.245
700	32.946	88.09	55.14	65.79	-904.341	-777.165	57.993
800	37.190	97.02	59.83	67.89	-903.523	-759.051	49.561
900	40.689	105.10	64.41	69.36	-902.644	-741.031	43.009
1000	43.611	112.47	68.86	70.40	-901.742	-723.132	37.773
1100	46.083	119.22	73.14	71.18	-900.838	-705.324	33.493
1200	48.202	125.44	77.24	71.81	-899.938	-687.574	29.929
1300	50.041	131.21	81.17	72.40	-899.045	-669.920	26.918
1400	51.657	136.60	84.94	73.01	-898.155	-652.343	24.339
1500	53.106	141.66	88.55	73.70	-897.246	-634.806	22.106
1600	54.419	146.44	92.02	74.52	-896.313	-617.337	20.154
1700	55.629	150.99	95.36	75.49	-895.844	-599.503	18.421
1800	56.764	155.34	98.58	76.66	-894.512	-579.166	16.807

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.0641 J/bar 20.641 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.3306 \times 10^{-2} - 7.7765 \times 10^{-2} T + 1.9237 \times 10^{-5} T^2 - 3.3753 \times 10^3 T^{-0.5} + 2.6036 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	285	101	101	COMPILED
				7-16-76

## STISHOVITE

FORMULA WEIGHT 60.085

SiO<sub>2</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	27.78	27.78	42.97	-861.318	-802.827	140.653
UNCERTAINTY		0.42	0.42		2.092	2.134	0.374
400	12.425	42.03	29.60	53.47	-861.526	-782.786	102.222
500	21.270	54.66	33.39	59.40	-861.211	-763.141	79.725
600	27.958	65.84	37.88	63.12	-860.631	-743.571	64.734
700	33.170	75.77	42.60	65.58	-859.918	-724.118	54.035
800	37.335	84.65	47.32	67.30	-859.141	-704.773	46.017
900	40.744	92.65	51.91	68.57	-858.328	-685.510	39.786
1000	43.574	99.93	56.36	69.56	-857.513	-666.363	34.867
1100	45.976	106.60	60.62	70.40	-856.689	-647.293	30.738
1200	48.045	112.76	64.72	71.18	-855.860	-628.280	27.348
1300	49.855	118.49	68.64	71.95	-855.021	-609.360	24.484
1400	51.464	123.85	72.39	72.77	-854.159	-590.497	22.032
1500	52.913	128.90	75.99	73.66	-853.270	-571.690	19.908
1600	54.240	133.69	79.45	74.66	-852.333	-552.957	18.052
1700	55.474	138.25	82.78	75.78	-901.842	-533.843	16.403
1800	56.636	142.61	85.97	77.03	-900.476	-512.216	14.864

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	1.4014 J/bar 14.014 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SILICON.... M. P. 1685 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.4740 \times 10^2 - 4.0271 \times 10^{-2} T + 1.2026 \times 10^{-5} T^2 - 1.5594 \times 10^3 T^{-0.5} - 2.8339 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	285	101	101	COMPILED 7-16-76
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SILICA GLASS

FORMULA WEIGHT 60.085

SiO<sub>2</sub>: Glass 298.15 to 1800 K.

FORMATION FROM THE ELEMENTS GIBBS							
TEMP.	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	47.40	47.40	37.94	-903.200	-850.559	149.015
UNCERTAINTY		0.21	0.21		2.092	2.134	0.374
400	11.875	61.01	49.13	53.16	-903.628	-832.480	108.711
500	20.896	73.69	52.79	59.95	-903.280	-814.725	85.114
600	27.738	84.97	57.23	63.64	-902.645	-797.063	69.391
700	33.041	94.96	61.92	65.93	-901.890	-779.523	58.169
800	37.259	103.88	66.62	67.53	-901.084	-762.100	49.760
900	40.689	111.91	71.22	68.77	-900.260	-744.776	43.226
1000	43.555	119.21	75.66	69.84	-899.414	-727.544	38.003
1100	45.989	125.91	79.92	70.82	-898.557	-710.402	33.734
1200	48.099	132.11	84.01	71.79	-897.677	-693.317	30.179
1300	49.958	137.90	87.94	72.77	-896.768	-676.340	27.176
1400	51.621	143.33	91.71	73.81	-895.821	-659.431	24.604
1500	53.139	148.46	95.32	74.90	-894.812	-642.572	22.376

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.7270 J/bar 27.270 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 74.639 - 7.2594 \times 10^{-3} T + 5.5704 \times 10^{-6} T^2 - 3.1140 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	52	285	148	COMPILED
	240	278	284	6- 8-76

## SARARIUM SESQUIOXIDE (MONOCLINIC)

FORMULA WEIGHT 348.798

Sm<sub>2</sub>O<sub>3</sub>: Alpha crystals 298.15 to 1195 K. Beta crystals 1195 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	151.04	151.04	113.36	-1822.970	-1796.690	314.774
UNCERTAINTY		4.20	4.20		2.010	2.020	0.354
400	30.500	186.16	155.66	124.86	-1821.626	-1704.896	222.638
500	50.050	214.75	164.70	131.15	-1820.503	-1675.853	175.076
600	63.947	239.07	175.12	135.51	-1819.774	-1647.001	143.385
700	74.423	260.22	185.80	138.95	-1819.280	-1618.240	120.755
800	82.677	278.97	196.29	141.90	-1818.864	-1589.548	103.787
900	89.411	295.84	206.43	144.58	-1818.451	-1560.898	90.593
1000	95.051	311.21	216.16	147.07	-1818.036	-1532.316	80.040
1100	99.889	325.34	225.45	149.45	-1817.660	-1503.764	71.408
1195	103.735	331.96	228.23	151.64	-1823.947	-1469.873	64.250
1195	104.487	332.72	228.23	154.41	-1823.049	-1469.873	64.250
1200	104.695	333.36	228.67	154.41	-1823.015	-1468.397	63.918
1300	108.519	345.72	237.20	154.41	-1822.342	-1438.868	57.815
1400	111.800	357.16	245.36	154.41	-1839.323	-1408.683	52.559
1500	114.637	367.81	253.17	154.41	-1839.404	-1377.899	47.983
1600	117.123	377.78	260.66	154.41	-1839.520	-1347.144	43.980
1700	119.316	387.14	267.82	154.41	-1839.672	-1316.387	40.448
1800	121.266	395.97	274.70	154.41	-1839.854	-1285.598	37.307

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	21.004 kJ	MOLAR VOLUME	4.5040 J/bar 45.040 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SARARIUM... ALPHA-BETA 1190, M. P. 1345 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.2841 \times 10^2 + 2.0545 \times 10^{-2} T - 1.8827 \times 10^{-4} T^2$$

(EQUATION VALID FROM 298 - 1195 K)

REFERENCE	210	235	235	COMPILED 5-18-76
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SAMARIUM SESQUIOXIDE (CUBIC) FORMULA WEIGHT 348.798

Sm<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1100 K.

TEMP. K	$\frac{H_T^0 - H_{298}^0}{T}$ / $\frac{S_T^0 - S_{298}^0}{T}$ - $\frac{-(G_T^0 - H_{298}^0)}{T}$ / $C_p^0$				FORMATION FROM THE ELEMENTS		
					GIBBS		
					ENTHALPY	FREE ENERGY	Log $\epsilon$
J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	0.00	---	112.37	---	---	---
UNCERTAINTY							
400	30.600	35.23	---	126.22	---	---	---
500	50.486	64.21	---	133.13	---	---	---
600	64.643	88.89	---	137.44	---	---	---
700	75.274	110.32	---	140.53	---	---	---
800	83.589	129.25	---	142.98	---	---	---
900	90.300	146.21	---	145.04	---	---	---
1000	95.871	161.59	---	146.87	---	---	---
1100	100.585	175.66	---	148.54	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.9100 J/bar 49.100 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SAMARIUM... ALPHA-BETA 1190, M. P. 1345 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.3702 \times 10^2 + 1.2365 \times 10^{-2} T - 2.5189 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1100 K)

REFERENCE 193 7 COMPILED 9-28-76

## CASSITERITE

FORMULA WEIGHT 150.689

SnO<sub>2</sub>: Crystals 298.15 to melting point 1903 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	52.30	52.30	52.59	-580.740	-519.902	91.085
UNCERTAINTY		1.25	1.25		0.628	0.753	0.132
400	15.050	69.57	54.52	64.03	-580.585	-499.109	65.177
500	25.468	84.54	59.07	69.82	-579.910	-478.820	50.022
600	33.185	97.62	64.43	73.50	-585.837	-457.383	39.819
700	39.144	109.16	70.02	76.18	-584.465	-436.079	32.541
800	43.912	119.48	75.57	78.34	-582.914	-414.986	27.096
900	47.844	128.81	80.97	80.18	-581.225	-394.088	22.872
1000	51.160	137.35	86.19	81.83	-579.426	-373.396	19.504
1100	54.018	145.22	91.20	83.36	-577.519	-352.888	16.757
1200	56.524	152.53	96.01	84.81	-575.508	-332.544	14.475
1300	58.753	159.38	100.63	86.19	-573.393	-312.392	12.552
1400	60.764	165.81	105.05	87.53	-571.170	-292.388	10.909
1500	62.589	171.90	109.31	88.84	-568.852	-272.557	9.491

MELTING POINT	1903	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.1550 J/bar 21.550 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

TIN..... M. P. 505 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 72.158 + 1.1726 \times 10^{-2} T - 2.0502 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	115	120	262	COMPILED 5-24-76
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STRONTIUM OXIDE

FORMULA WEIGHT 103.619

SrO: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	55.52	55.52	45.41	-590.490	-560.353	98.172
UNCERTAINTY		0.42	0.42		0.920	0.930	0.163
400	12.000	69.35	57.35	48.55	-590.010	-549.580	71.768
500	19.518	80.41	60.89	50.52	-589.509	-539.534	56.365
600	24.813	89.75	64.94	52.00	-589.066	-529.573	46.104
700	28.786	97.86	69.07	53.21	-588.740	-519.692	38.780
800	31.905	105.04	73.14	54.26	-588.581	-509.841	33.289
900	34.444	111.48	77.04	55.20	-589.309	-499.921	29.015
1000	36.562	117.34	80.78	56.07	-589.241	-490.001	25.595
1100	38.373	122.73	84.36	56.89	-597.162	-479.627	22.776
1200	39.948	127.71	87.76	57.66	-596.723	-468.953	20.413
1300	41.339	132.35	91.01	58.41	-596.228	-458.324	18.416
1400	42.586	136.71	94.12	59.13	-595.674	-447.750	16.706
1500	43.711	140.81	97.10	59.83	-595.067	-437.192	15.224
1600	44.740	144.70	99.96	60.52	-594.402	-426.698	13.930
1700	45.688	148.39	102.70	61.19	-729.968	-412.468	12.674
1800	46.568	151.90	105.33	61.85	-727.763	-393.827	11.429

MELTING POINT	2938	K	BOILING POINT	K
ENTHALPY OF MELTING	75.300	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	8.673	kJ	MOLAR VOLUME	2.0686 J/bar 20.686 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

STRONTIUM.. ALPHA-GAMMA 828, H. P. GAMMA 1041, B. P. 1652 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 55.667 + 5.4617 \times 10^{-3} T - 1.5122 \times 10^{-6} T^2 + 2.7805 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	33	33	24	COMPILED
	155			6- 8-76

## DITANTALUM PENTOXIDE (BETA)

FORMULA WEIGHT 441.893

Ta<sub>2</sub>O<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS					GIBBS		Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol		
298.15	0.000	143.13	143.13	135.03	-2045.976	-1910.984	334.798	
UNCERTAINTY		1.26	1.26		4.184	4.200	0.736	
400	36.425	185.06	148.63	149.51	-2044.204	-1865.110	243.559	
500	59.960	219.41	159.45	158.20	-2041.680	-1820.620	190.200	
600	76.878	248.84	171.96	164.48	-2038.723	-1776.682	154.675	
700	89.760	274.58	184.82	169.45	-2035.483	-1733.265	129.338	
800	99.987	297.48	197.49	173.63	-2032.029	-1690.313	110.367	
900	108.378	318.15	209.77	177.29	-2028.397	-1647.805	95.637	
1000	115.435	337.00	221.57	180.58	-2024.610	-1605.720	83.875	
1100	121.496	354.36	232.86	183.61	-2020.684	-1564.030	74.270	
1200	126.792	370.45	243.66	186.44	-2016.633	-1522.671	66.280	
1300	131.483	385.48	254.00	189.12	-2012.458	-1481.694	59.535	
1400	135.693	399.59	263.90	191.67	-2008.171	-1441.017	53.765	
1500	139.505	412.90	273.39	194.12	-2003.778	-1400.658	48.775	
1600	142.992	425.50	282.51	196.49	-1999.284	-1360.620	44.420	
1700	146.207	437.48	291.27	198.79	-1994.692	-1320.838	40.585	
1800	149.191	448.90	299.71	201.03	-1990.012	-1281.334	37.184	

MELTING POINT	2058	K	BOILING POINT	K
ENTHALPY OF MELTING	120.100	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	23.041	kJ	MOLAR VOLUME	5.3170 J/bar 53.170 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_P^0 = 1.8972 \times 10^2 + 1.6639 \times 10^{-2} T - 7.7377 \times 10^2 T^{-0.5} - 1.3090 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	33	33	33	COMPILED
	189			6- 2-76



TERBIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 365.849

Tb<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol
298.15	0.000	156.90	156.90	127.27	-1865.230	-1776.553	311.246
UNCERTAINTY		4.20	4.20		8.370	8.400	1.472
400	30.725	192.31	161.58	124.12	-1863.256	-1746.554	228.078
500	49.850	220.48	170.63	128.21	-1860.889	-1717.634	179.441
600	63.168	244.13	180.96	131.19	-1858.521	-1689.204	147.059
700	73.073	264.55	191.48	133.79	-1856.269	-1661.172	123.959
800	80.819	282.58	201.76	136.27	-1854.173	-1633.441	106.653
900	87.122	298.77	211.65	138.75	-1852.237	-1605.961	93.208
1000	92.405	313.52	221.12	141.25	-1850.472	-1578.702	82.463
1100	96.961	327.10	230.14	143.80	-1848.857	-1551.593	73.679
1200	100.972	339.73	238.76	146.39	-1847.389	-1524.655	66.367
1300	104.567	351.55	246.98	149.04	-1846.054	-1497.797	60.183
1400	107.836	362.69	254.85	151.72	-1844.857	-1471.071	54.887
1500	110.855	373.25	262.39	154.45	-1843.761	-1444.386	50.298
1600	113.666	383.31	269.64	157.21	-1851.521	-1417.465	46.276
1700	116.310	392.92	276.61	160.01	-1871.000	-1389.430	42.692
1800	118.816	402.15	283.33	162.84	-1869.729	-1361.053	39.497

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.6480 J/bar 46.480 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

TERBIUM....ALPHA-BETA 1560, H. P. 1630 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 88.639 + 3.2326 \times 10^{-2} T + 7.0601 \times 10^{-2} T^{-0.5} - 2.0403 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	200	281	235	COMPILED 8-18-76
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## TERBIUM OXIDE

FORMULA WEIGHT 186.348

TbO<sub>1.714</sub>: Crystals 298.15 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	80.75	80.75	57.37	-953.950	-938.980	164.506
UNCERTAINTY		4.20	4.20		4.180	4.200	0.736
400	15.925	99.12	83.19	63.92	-953.061	-886.743	115.797
500	25.794	113.67	87.88	66.58	-951.996	-870.276	90.918
600	32.815	126.04	93.23	69.25	-950.847	-854.034	74.351
700	38.210	136.92	98.71	71.91	-949.636	-838.002	62.533
800	42.589	146.69	104.10	74.57	-948.373	-822.131	53.680
900	46.289	155.63	109.34	77.24	-947.057	-806.433	46.804
1000	49.518	163.90	114.38	79.90	-945.684	-790.876	41.311

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

TERBIUM.....ALPHA-BETA 1560, N. P. 1630 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 53.269 + 2.6629 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	200	281	235	COMPILED 8-18-76
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TERBIUM OXIDE

FORMULA WEIGHT 187.916

TbO<sub>1.812</sub>: Crystals 298.15 to 900 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	81.17	81.17	61.96	-960.230	-942.180	165.067
UNCERTAINTY		4.20	4.20		4.180	4.200	0.736
400	15.825	99.40	83.57	65.11	-959.530	-889.131	116.109
500	26.090	114.36	88.27	68.84	-958.427	-871.645	91.060
600	33.448	127.16	93.71	71.51	-957.200	-854.401	74.383
700	39.046	138.35	99.30	73.69	-955.944	-837.371	62.486
800	43.497	148.32	104.82	75.60	-954.702	-820.516	53.574
900	47.167	157.32	110.15	77.35	-953.490	-803.805	46.652

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	J/bar

TRANSITIONS IN REFERENCE STATE ELEMENTS

TERBIUM....ALPHA-BETA 1560, H. P. 1630 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 65.863 + 1.4175 \times 10^{-2} T - 1.0273 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	200	281	235	COMPILED
				8-18-76

## THORIANITE

FORMULA WEIGHT 264.037

ThO<sub>2</sub>: Crystals 298.15 to 1200 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	65.23	65.23	61.76	-1226.410	-1168.775	204.765
UNCERTAINTY		0.21	0.21		3.510	3.510	0.615
400	16.600	84.34	67.74	67.82	-1225.646	-1149.190	150.069
500	27.180	99.84	72.66	70.95	-1224.688	-1130.188	118.070
600	34.655	112.96	78.30	72.99	-1223.705	-1111.373	96.754
700	40.244	124.33	84.09	74.52	-1222.764	-1092.732	81.541
800	44.609	134.37	89.76	75.78	-1221.890	-1074.218	70.140
900	48.133	143.36	95.23	76.88	-1221.092	-1055.807	61.278
1000	51.060	151.51	100.45	77.88	-1220.372	-1037.472	54.192
1100	53.541	163.98	110.44	78.82	-1219.734	-1024.726	48.660
1200	55.685	165.88	110.19	79.72	-1219.175	-1001.027	43.574

MELTING POINT	3493 K	BOILING POINT	K
ENTHALPY OF MELTING		ENTHALPY OF VAPORIZATION	
$H_{298}^0 - H_0^0$	10.562 kJ	MOLAR VOLUME	2.6373 J/bar 26.373 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

THORIUM.... ALPHA-BETA 1636, M. P. BETA 2028 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 71.379 + 7.5563 \times 10^{-3} T - 1.0529 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	260	215	215	COMPILED
	240			6-11-76

TITANIUM OXIDE FORMULA WEIGHT 63.899

TiO: Alpha crystals 298.15 to 1265 K. Beta crystals 1265 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	34.77	34.77	39.96	-542.660	-513.312	89.931
UNCERTAINTY		2.10	2.10		12.550	12.550	2.199
400	11.225	47.68	36.45	46.84	-542.300	-503.326	65.728
500	18.614	58.42	39.81	49.16	-541.704	-493.654	51.572
600	23.828	67.51	43.68	50.62	-541.084	-484.099	42.145
700	27.760	75.42	47.66	52.11	-540.461	-474.647	35.419
800	30.910	82.49	51.58	53.87	-539.814	-465.290	30.380
900	33.578	88.96	55.38	55.95	-539.103	-456.015	26.467
1000	35.929	94.97	59.04	58.33	-538.304	-446.824	23.340
1100	38.084	100.65	62.57	60.98	-537.378	-437.718	20.786
1200	40.110	106.08	65.97	63.86	-540.351	-428.553	18.655
1265	41.330	109.34	68.01	65.84	-539.348	-422.719	17.455
1265	41.340	109.35	68.01	64.04	-539.335	-422.719	17.455
1300	41.983	111.20	69.22	64.67	-538.722	-419.252	16.846
1400	43.664	116.06	72.40	66.46	-537.108	-410.128	15.302
1500	45.246	120.71	75.46	68.24	-535.425	-401.115	13.968
1600	46.739	125.17	78.43	70.03	-533.683	-392.219	12.805
1700	48.162	129.47	81.31	71.82	-531.879	-383.444	11.782
1800	49.526	133.62	84.09	73.60	-530.011	-374.743	10.875

MELTING POINT	2023 K	BOILING POINT	K
ENTHALPY OF MELTING	41.800 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	1.3000 J/bar 13.000 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = - 52.663 + 5.0219 \times 10^{-2} T + 2.0349 \times 10^{-5} T^2 - 3.5732 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1265 K)

$$C_P^0 = 41.443 + 1.7867 \times 10^{-2} T$$

(EQUATION VALID FROM 1265 - 1800 K)

REFERENCE 176 33 33 COMPILED  
8-11-76

## RUTILE

FORMULA WEIGHT 79.899

TiO<sub>2</sub>: Crystals 298.15 to melting point 2103 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	50.29	50.29	55.10	-944.750	-889.446	155.828
UNCERTAINTY		0.17	0.17		1.260	1.030	0.180
400	14.875	67.42	52.55	61.16	-944.442	-870.590	113.688
500	24.502	81.46	56.96	64.54	-943.894	-852.189	89.028
600	31.380	93.45	62.07	66.89	-943.269	-833.907	72.598
700	36.591	103.90	67.31	68.77	-942.623	-815.727	60.871
800	40.716	113.19	72.47	70.39	-941.979	-797.643	52.081
900	44.100	121.57	77.47	71.85	-941.342	-779.630	45.249
1000	46.940	129.21	82.27	73.22	-940.730	-761.700	39.787
1100	49.389	136.25	86.86	74.53	-940.132	-743.826	35.321
1200	51.537	142.79	91.25	75.80	-943.603	-725.851	31.596
1300	53.452	148.91	95.46	77.04	-942.572	-707.753	28.438
1400	55.179	154.66	99.48	78.26	-941.557	-689.725	25.734
1500	56.759	160.10	103.34	79.46	-940.550	-671.765	23.393
1600	58.214	165.27	107.06	80.64	-939.556	-653.892	21.347
1700	59.568	170.19	110.62	81.82	-938.571	-636.073	19.544
1800	60.837	174.90	114.06	82.99	-937.594	-618.292	17.942

MELTING POINT	2103	K	BOILING POINT		K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION		kJ
$H_{298}^0 - H_0^0$	8.669	kJ	MOLAR VOLUME	1.8820	J/bar
				18.820	cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 63.079 + 1.1307 \times 10^{-2} T - 5.6160 T^{-0.5} - 9.8626 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	33	33	33	COMPILED
	176		215	6-21-76

ANATASE

FORMULA WEIGHT 79.899

TiO<sub>2</sub>: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	49.91	49.91	55.27	-938.720	-883.303	154.752
UNCERTAINTY		0.29	0.29		2.090	2.090	0.366
400	15.475	67.70	52.22	64.70	-938.172	-864.432	112.884
500	25.756	82.61	56.85	68.60	-937.237	-846.107	88.393
600	33.085	95.32	62.24	70.69	-936.216	-827.976	72.082
700	38.560	106.32	67.76	72.07	-935.215	-810.013	60.444
800	42.819	116.02	73.20	73.15	-934.267	-792.195	51.725
900	46.244	124.69	78.45	74.10	-933.382	-774.479	44.950
1000	49.073	132.54	83.47	75.01	-932.567	-756.867	39.535
1100	51.471	139.74	88.27	75.90	-931.812	-739.345	35.109
1200	53.545	146.38	92.84	76.81	-935.164	-721.720	31.416
1300	55.371	152.56	97.19	77.74	-934.047	-703.973	28.286

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.0520 J/bar 20.520 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS  
 TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 43.961 + 1.3738 \times 10^{-2} T + 6.2937 \times 10^{-5} T^2 - 2.5953 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	176	33	33	COMPILED 6-14-76
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## DITITANIUM TRIOXIDE

FORMULA WEIGHT 143.798

Ti<sub>2</sub>O<sub>3</sub>: Alpha crystals 298.15 to 470 K. Beta crystals 470 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS							
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	77.25	77.25	95.81	-1520.884	-1433.903	251.215	
UNCERTAINTY		0.21	0.21		8.368	8.370	1.466	
400	27.017	108.27	81.26	117.53	-1519.849	-1404.293	183.383	
470	38.797	129.60	87.80	132.47	-1519.299	-1384.751	153.899	
470	44.259	132.05	87.80	127.69	-1516.732	-1384.751	153.899	
500	49.622	139.36	89.74	130.29	-1515.819	-1375.804	143.730	
600	63.625	163.71	100.08	136.46	-1512.777	-1348.080	117.361	
700	74.326	185.05	110.72	140.32	-1509.576	-1320.877	98.566	
800	82.749	203.97	121.22	142.96	-1506.369	-1294.141	84.499	
900	89.556	220.93	131.37	144.88	-1503.229	-1267.789	73.581	
1000	95.161	236.27	141.11	146.35	-1500.216	-1241.796	64.865	
1100	99.871	250.28	150.41	147.54	-1497.346	-1216.098	57.748	
1200	103.885	263.16	159.28	148.52	-1502.743	-1190.341	51.814	
1300	107.352	275.08	167.73	149.36	-1499.276	-1164.448	46.788	
1400	110.379	286.18	175.80	150.10	-1495.989	-1138.821	42.490	
1500	113.050	296.56	183.51	150.76	-1492.881	-1113.411	38.773	
1600	115.426	306.30	190.87	151.36	-1489.958	-1088.206	35.526	
1700	117.556	315.50	197.94	151.92	-1487.219	-1063.214	32.669	
1800	119.481	324.20	204.72	152.44	-1484.667	-1038.321	30.131	

MELTING POINT	2115 K	BOILING POINT	K
ENTHALPY OF MELTING	104.600 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	14.088 kJ	MOLAR VOLUME	3.1430 J/bar 31.430 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

TITANIUM... ALPHA-BETA 1155, H. P. 1943 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.4861 \times 10^2 + 3.2861 \times 10^{-3} T - 27.026 T^{-0.5} - 4.6881 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 470 - 1800 K)

REFERENCE	33	33	33	COMPILED
	176			8- 2-76



TRITITANIUM PENTOXIDE (ALPHA)

FORMULA WEIGHT 223.697

Ti<sub>3</sub>O<sub>5</sub>: Alpha crystals 298.15 to 450 K. Beta crystals 450 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	129.37	129.37	154.81	-2459.150	-2317.411	406.003
UNCERTAINTY		1.67	1.67		4.180	4.600	0.806
400	43.377	179.23	135.85	182.84	-2457.213	-2269.219	296.331
450	59.739	203.71	143.97	196.52	-2456.285	-2246.952	260.821
450	87.489	231.45	143.97	168.45	-2442.784	-2246.952	260.821
500	97.272	248.33	151.06	178.31	-2441.655	-2223.690	232.308
600	111.947	282.08	170.13	191.15	-2439.397	-2180.290	189.812
700	123.857	312.17	188.31	198.90	-2436.657	-2137.316	159.489
800	133.571	339.08	205.51	203.92	-2433.779	-2094.751	136.774
900	141.589	363.31	221.72	207.37	-2430.947	-2052.524	119.126
1000	148.298	385.29	236.99	209.83	-2428.265	-2010.625	105.025
1100	153.979	405.38	251.40	211.66	-2425.803	-1968.984	93.500
1200	158.846	423.86	265.01	213.04	-2435.754	-1927.092	83.884
1300	163.058	440.96	277.90	214.12	-2432.433	-1884.847	75.734
1400	166.736	456.86	290.12	214.98	-2429.412	-1842.840	68.758
1500	169.977	471.71	301.73	215.67	-2426.695	-1801.015	62.717
1600	172.851	485.65	312.80	216.24	-2424.293	-1759.405	57.439
1700	175.416	498.77	323.35	216.70	-2422.210	-1717.943	52.786
1800	177.722	511.17	333.45	217.10	-2420.450	-1676.528	48.652

MELTING POINT	2050	K	BOILING POINT	K
ENTHALPY OF MELTING	172.000	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	5.2690 J/bar 52.690 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.2034 \times 10^2 - 1.0507 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 450 - 1800 K)

REFERENCE	176	33	33	COMPILED 8-17-76
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## TETRATITANIUM HEPTOXIDE

FORMULA WEIGHT 303.596

Ti<sub>4</sub>O<sub>7</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	198.74	198.74	208.49	-3404.520	-3213.166	562.936
UNCERTAINTY		12.00	12.00		6.280	6.280	1.100
400	57.650	265.05	207.40	240.78	-3402.516	-3148.030	411.092
500	96.214	320.86	224.65	258.73	-3398.949	-3084.814	322.270
600	124.345	369.14	244.80	270.54	-3394.675	-3022.372	263.122
700	145.864	411.52	265.66	279.02	-3390.109	-2960.687	220.930
800	162.929	449.21	286.28	285.48	-3385.465	-2899.653	189.329
900	176.844	483.14	306.30	290.61	-3380.869	-2839.168	164.782
1000	188.435	513.99	325.56	294.82	-3376.418	-2779.238	145.173
1100	198.272	542.26	343.99	298.36	-3372.161	-2719.729	129.150
1200	206.742	568.35	361.61	301.38	-3368.347	-2659.973	115.786
1300	214.125	592.58	378.46	304.01	-3378.725	-2599.843	104.463
1400	220.629	615.20	394.57	306.33	-3373.389	-2540.137	94.774
1500	226.413	636.40	409.99	308.39	-3368.349	-2480.769	86.388
1600	231.594	656.37	424.78	310.24	-3363.622	-2421.790	79.064
1700	236.271	675.22	438.95	311.91	-3359.215	-2363.092	72.609
1800	240.516	693.10	452.58	313.44	-3355.142	-2304.572	66.877

MELTING POINT	1950	K	BOILING POINT	K
ENTHALPY OF MELTING	226.000	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 3.6004 \times 10^2 + 5.2682 \times 10^{-4} T - 1.9739 \times 10^3 T^{-0.5} - 3.3236 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	33	33	33	COMPILED
				5-19-76

THULIUM SESQUIOXIDE

FORMULA WEIGHT 385.867

Tm<sub>2</sub>O<sub>3</sub>: Alpha crystals 298.15 to 1680 K. Beta crystals 1680 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
					kJ/mol	kJ/mol	
298.15	0.000	139.75	139.75	112.88	-1888.660	-1794.446	314.381
UNCERTAINTY		0.85	0.85		0.850	0.850	0.149
400	30.125	174.29	144.16	121.43	-1886.546	-1762.492	230.159
500	48.830	201.87	153.04	125.43	-1884.107	-1731.767	180.917
600	61.803	224.95	163.15	127.73	-1881.666	-1701.525	148.132
700	71.336	244.76	173.42	129.23	-1879.363	-1671.687	124.743
800	78.642	262.09	183.45	130.30	-1877.238	-1642.162	107.223
900	84.433	277.49	193.06	131.13	-1875.307	-1612.885	93.610
1000	89.135	291.34	202.20	131.80	-1873.558	-1583.828	82.731
1100	93.039	303.93	210.89	132.37	-1871.993	-1554.940	73.838
1200	96.337	315.47	219.13	132.87	-1870.600	-1526.170	66.433
1300	99.165	326.12	226.95	133.32	-1869.366	-1497.514	60.171
1400	101.621	336.02	234.40	133.73	-1868.287	-1468.979	54.809
1500	103.774	345.26	241.49	134.12	-1867.351	-1440.481	50.162
1600	105.682	353.93	248.25	134.49	-1866.553	-1412.049	46.099

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	20.878 kJ	MOLAR VOLUME	4.3420 J/bar 43.420 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

THULIUM.... M. P. 1818 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.3063 \times 10^2 + 2.8191 \times 10^{-3} T - 1.6528 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	207	235	235	COMPILED 5-19-76
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## URANINITE

FORMULA WEIGHT 270.028

UO<sub>2</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	77.03	77.03	63.60	-1084.910	-1031.770	180.763
UNCERTAINTY		0.24	0.24		1.000	1.000	0.175
400	17.375	97.01	79.63	71.65	-1083.903	-1013.679	132.373
500	28.644	113.46	84.82	75.51	-1082.676	-996.276	104.081
600	36.672	127.45	90.78	77.96	-1081.493	-979.103	85.239
700	42.707	139.62	96.91	79.83	-1080.491	-962.128	71.795
800	47.449	150.38	102.93	81.42	-1079.744	-945.264	61.720
900	51.311	160.06	108.75	82.90	-1079.312	-928.481	53.888
1000	54.536	168.87	114.33	84.31	-1081.664	-911.574	47.616
1100	57.306	176.97	119.66	85.70	-1085.478	-894.364	42.470
1200	59.729	184.48	124.75	87.07	-1084.218	-877.038	38.177
1300	61.885	191.51	129.62	88.45	-1082.857	-859.829	34.549
1400	63.836	198.11	134.27	89.84	-1081.388	-842.730	31.443
1500	65.613	204.36	138.75	91.23	-1089.249	-825.129	28.734
1600	67.258	210.29	143.03	92.64	-1088.524	-807.548	26.364
1700	68.792	215.95	147.16	94.05	-1087.680	-790.027	24.275
1800	70.236	221.36	151.12	95.48	-1086.716	-772.526	22.418

MELTING POINT	3151	K	BOILING POINT	K
ENTHALPY OF MELTING		KJ	ENTHALPY OF VAPORIZATION	KJ
$H_{298}^0 - H_0^0$		KJ	MOLAR VOLUME	2.4618 J/bar 24.618 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS				

URANIUM.... ALPHA-BETA 941, BETA-GAMMA 1048, M. P. 1405 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 58.454 + 1.6057 \times 10^{-2} T + 3.6889 \times 10^{-5} T^2 - 1.8672 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	77	110	41	COMPILED
	60	215	215	7-21-76

URANIUM TRIOXIDE (GAMMA)

FORMULA WEIGHT 286.027

$\gamma$ -UO<sub>3</sub>: Crystals 298.15 to 900 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	98.62	98.62	84.72	-1223.800	-1146.461	200.856
UNCERTAINTY		0.25	0.25		0.800	1.000	0.175
400	22.025	124.00	101.98	88.55	-1222.445	-1120.243	146.289
500	35.736	144.21	108.47	92.53	-1221.064	-1094.864	114.380
600	45.467	161.36	115.89	95.54	-1219.732	-1069.747	93.130
700	52.773	176.25	123.48	97.53	-1218.588	-1044.848	77.968
800	58.447	189.35	130.90	98.68	-1217.754	-1020.078	66.605
900	62.944	201.01	138.07	99.14	-1217.351	-995.402	57.772

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.5560 J/bar 35.560 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

URANIUM.... ALPHA-BETA 941, BETA-GAMMA 1048, H. P. 1405 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.1500 \times 10^2 - 3.8496 \times 10^{-2} T - 2.5272 \times 10^3 T^{-0.5} + 2.4500 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	170	112	215	COMPILED
		215		6- 8-76

VANADIUM MONOXIDE FORMULA WEIGHT 66.941

VO: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	39.01	39.01	45.50	-431.790	-404.219	70.818
UNCERTAINTY		0.85	0.85		6.280	6.280	1.100
400	12.075	52.91	40.84	49.10	-431.078	-394.900	51.569
500	19.746	64.16	44.41	51.71	-430.213	-385.958	40.321
600	25.257	73.78	48.52	53.85	-429.225	-377.196	32.838
700	29.479	82.23	52.75	55.73	-428.146	-368.611	27.506
800	32.867	89.78	56.91	57.44	-426.998	-360.178	23.517
900	35.689	96.64	60.95	59.03	-425.795	-351.896	20.424
1000	38.097	102.94	64.84	60.55	-424.555	-343.755	17.956
1100	40.205	108.78	68.58	62.00	-423.284	-335.735	15.943
1200	42.081	114.23	72.15	63.41	-421.995	-327.825	14.270
1300	43.775	119.36	75.59	64.79	-420.699	-320.027	12.859
1400	45.321	124.21	78.89	66.13	-419.410	-312.338	11.654
1500	46.755	128.82	82.07	67.45	-418.126	-304.741	10.612
1600	48.089	133.22	85.13	68.76	-416.865	-297.225	9.703
1700	49.343	137.42	88.08	70.04	-415.635	-289.776	8.904
1800	50.528	141.46	90.93	71.31	-414.445	-282.415	8.196

MELTING POINT	2063	K	BOILING POINT	K
ENTHALPY OF MELTING	54.400	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	1.0260 J/bar 10.260 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

VANADIUM... M. P. 2175 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 55.932 + 1.1245 \times 10^{-2} T - 2.0393 \times 10^{-5} T^{0.5} - 1.8079 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	115	33	33	COMPILED
	191			6- 2-76

KARELIANITE

FORMULA WEIGHT 149.881

V<sub>2</sub>O<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	98.07	98.07	104.96	-1218.800	-1139.052	199.558
UNCERTAINTY		1.25	1.25		6.280	6.500	1.139
400	28.625	131.01	102.38	117.82	-1217.098	-1112.044	145.219
500	47.090	157.98	110.89	123.52	-1214.891	-1086.036	113.458
600	60.143	180.83	120.69	127.11	-1212.518	-1060.481	92.323
700	69.920	200.65	130.73	129.99	-1210.092	-1035.337	77.258
800	77.596	218.18	140.58	132.66	-1207.647	-1010.531	65.981
900	83.867	233.96	150.09	135.32	-1205.189	-986.030	57.228
1000	89.144	248.36	159.22	138.04	-1202.727	-961.817	50.240
1100	93.715	261.65	167.93	140.84	-1200.251	-937.846	44.535
1200	97.763	274.03	176.27	143.74	-1197.763	-914.101	39.790
1300	101.415	285.65	184.24	146.73	-1195.262	-890.555	35.783
1400	104.757	296.63	191.87	149.80	-1192.759	-867.217	32.356
1500	107.867	307.08	199.21	152.95	-1190.239	-844.069	29.393
1600	110.786	317.05	206.26	156.17	-1187.722	-821.058	26.805
1700	113.552	326.62	213.07	159.46	-1185.211	-798.232	24.527
1800	116.194	335.82	219.63	162.80	-1182.714	-775.536	22.506

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.9850 J/bar 29.850 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

VANADIUM... M. P. 2175 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 57.989 + 4.1200 \times 10^{-2} T + 1.3510 \times 10^{-5} T^2 - 3.8718 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	38	33	33	COMPILED 6-21-76
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## DIVANADIUM TETROXIDE

FORMULA WEIGHT 165.880

V<sub>2</sub>O<sub>4</sub>: Crystals 298.15 to 1600 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	103.52	103.52	115.40	-1427.162	-1318.457	230.989
UNCERTAINTY		2.09	2.09		6.276	6.500	1.139
400	54.700	140.96	86.26	134.24	-1416.542	-1272.694	166.198
500	71.516	171.89	100.37	142.77	-1414.084	-1237.009	129.230
600	83.905	198.47	114.57	148.61	-1411.249	-1201.855	104.631
700	93.471	221.72	128.25	152.93	-1408.222	-1167.198	87.098
800	101.120	242.37	141.25	156.27	-1405.110	-1132.974	73.976
900	107.400	260.93	153.53	158.95	-1401.990	-1099.131	63.792
1000	112.670	277.80	165.13	161.16	-1398.910	-1065.650	55.664
1100	117.165	293.25	176.08	163.02	-1395.918	-1032.467	49.028
1200	121.054	307.50	186.45	164.61	-1393.051	-999.547	43.509
1300	124.458	320.73	196.27	165.99	-1390.336	-966.861	38.849
1400	127.471	333.08	205.61	167.19	-1387.800	-934.396	34.863
1500	130.153	344.65	214.50	168.25	-1385.477	-902.102	31.414
1600	132.564	355.54	222.98	169.19	-1383.382	-869.942	28.401

MELTING POINT	1818	K	BOILING POINT	K
ENTHALPY OF MELTING	112.068	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	18.100	kJ	MOLAR VOLUME	J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

VANADIUM... H. P. 2175 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.0206 \times 10^2 - 1.1343 \times 10^{-3} T - 1.2270 \times 10^{-5} T^2 - 9.6254 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	38	33	33	COMPILED 5-19-76
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DIVANADIUM PENTOXIDE

FORMULA WEIGHT 181.880

V<sub>2</sub>O<sub>5</sub>: Crystals 298.15 to melting point 943 K. Liquid 943 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	130.54	130.54	130.60	-1550.590	-1419.435	248.680
UNCERTAINTY		2.09	2.09		6.276	6.300	1.104
400	38.650	175.11	136.46	154.30	-1547.902	-1374.940	179.550
500	62.276	210.07	147.79	159.26	-1545.176	-1332.016	139.155
600	78.852	239.55	160.70	164.21	-1542.335	-1289.648	112.274
700	91.401	265.23	173.83	169.16	-1539.352	-1247.767	93.110
800	101.431	288.15	186.72	174.12	-1536.208	-1206.325	78.765
900	109.778	308.94	199.16	179.07	-1532.897	-1165.275	67.631
943	113.445	317.32	203.87	181.20	-1530.841	-1147.106	63.541
943	181.865	385.74	203.87	188.33	-1466.321	-1147.106	63.541
1000	182.305	396.04	213.74	189.05	-1464.050	-1127.240	58.881
1100	182.966	414.11	231.14	190.06	-1460.065	-1093.754	51.938
1200	183.590	430.68	247.09	190.82	-1456.311	-1060.617	46.168
1300	184.170	445.98	261.81	191.41	-1452.807	-1027.785	41.297
1400	184.707	460.18	275.47	191.89	-1449.577	-995.221	37.132
1500	185.197	473.43	288.23	192.27	-1446.643	-962.878	33.531

MELTING POINT	943 K	BOILING POINT	K
ENTHALPY OF MELTING	64.520 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	21.506 kJ	MOLAR VOLUME	5.3940 J/bar 53.940 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

VANADIUM... H. P. 2175 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.3449 \times 10^2 + 4.9532 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 943 K)

$$C_P^0 = 1.9484 \times 10^2 - 5.7891 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 943 - 1500 K)

REFERENCE	837	710	710	COMPILED
				6- 7-76

## TUNGSTEN DIOXIDE

FORMULA WEIGHT 215.849

WO<sub>2</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	50.53	50.53	55.74	-589.690	-533.858	93.530
UNCERTAINTY		0.29	0.29		0.880	0.960	0.168
400	15.150	67.96	52.81	63.02	-589.172	-514.848	67.233
500	25.282	82.62	57.34	68.29	-588.191	-496.371	51.856
600	32.762	95.41	62.65	71.77	-586.919	-478.127	41.625
700	38.506	106.65	68.14	74.02	-585.495	-460.111	34.334
800	43.045	116.64	73.60	75.53	-583.996	-442.300	28.879
900	46.722	125.60	78.88	76.64	-582.464	-424.667	24.647
1000	49.761	133.73	83.97	77.63	-580.924	-407.224	21.271
1100	52.342	141.18	88.84	78.68	-579.361	-389.930	18.516
1200	54.587	148.07	93.48	79.92	-577.761	-372.765	16.226
1300	56.593	154.53	97.94	81.48	-576.091	-355.754	14.294
1400	58.436	160.64	102.20	83.42	-574.316	-338.892	12.644
1500	60.181	166.47	106.29	85.81	-572.380	-322.120	11.217
1600	61.870	172.10	110.23	88.70	-570.245	-305.525	9.974
1700	63.547	177.58	114.03	92.14	-567.850	-289.050	8.881
1800	65.245	182.96	117.72	96.16	-565.138	-272.728	7.914

MELTING POINT	K	BOILING POINT	1997	K
kJ	HOLAR VOLUME	1.9920 J/bar	19.920	cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

TUNGSTEN... M. P. 3680 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.7572 \times 10^2 - 0.12311 T + 3.9685 \times 10^{-5} T^2 - 3.7038 \times 10^3 T^{-0.5} + 2.4616 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	140	247	247	COMPILED
				7- 2-76

TUNGSTEN TRIOXIDE

FORMULA WEIGHT 231.848

WO<sub>3</sub>: Crystals (monoclinic) 298.15 to 593 K. Orthorhombic crystals 593 to 1050 K. Tetragonal crystals 1050 to melting point 1745 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	75.91	75.91	73.14	-842.909	-764.062	133.861
UNCERTAINTY		1.26	1.26		0.837	0.879	0.154
400	19.875	98.79	78.91	82.19	-842.013	-737.247	96.275
500	33.010	117.85	84.84	88.56	-840.590	-711.210	74.300
600	42.667	134.42	91.75	93.07	-838.821	-685.494	59.678
700	50.100	149.01	98.91	96.15	-836.851	-660.101	49.258
800	55.991	161.99	106.00	98.15	-834.777	-634.989	41.461
900	60.744	173.63	112.89	99.32	-832.682	-610.139	35.412
1000	64.635	184.12	119.48	99.85	-830.616	-585.516	30.584
1050	66.374	189.36	122.98	99.91	-829.509	-573.510	28.531
1050	67.894	190.88	122.98	99.23	-827.916	-573.510	28.531
1100	69.368	195.24	125.87	99.78	-826.951	-561.180	26.648
1200	71.948	203.97	132.02	100.88	-825.021	-537.099	23.379
1300	74.216	212.09	137.87	101.98	-823.068	-513.187	20.620
1400	76.236	219.68	143.44	103.09	-821.094	-489.434	18.261
1500	78.066	226.83	148.76	104.19	-819.075	-465.795	16.220
1600	79.733	233.59	153.86	105.29	-817.025	-442.329	14.441
1700	81.269	240.01	158.74	106.40	-814.933	-418.978	12.874

MELTING POINT	1745	K	BOILING POINT	K
ENTHALPY OF MELTING	73.429	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	12.339	kJ	MOLAR VOLUME	3.1610 J/bar 31.610 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

TUNGSTEN... N. P. 3680 K.

HEAT CAPACITY EQUATIONS

$$C_p^0 = 2.1388 \times 10^2 - 3.4684 \times 10^{-2} T - 2.5610 \times 10^3 T^{-0.5} + 1.6374 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1050 K)

$$C_p^0 = 87.642 + 1.1033 \times 10^{-2} T$$

(EQUATION VALID FROM 1050 - 1745 K)

REFERENCE	140	247	247	COMPILED 8-12-76
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## YTTRIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 225.810

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$Y_2O_3$ : Alpha crystals 298.15 to 1330 K. Beta crystals 1330 to 1800 K.

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TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY	FREE ENERGY	Log $K_f$
					kJ/mol	kJ/mol	
298.15	0.000	99.08	99.08	102.84	-1905.310	-1816.609	318.264
UNCERTAINTY		4.20	4.20		2.260	2.400	0.420
400	27.650	130.91	103.26	112.95	-1904.246	-1786.448	233.287
500	45.256	156.71	111.45	117.97	-1902.782	-1757.172	183.571
600	57.652	178.51	120.86	121.09	-1901.211	-1728.186	150.453
700	66.881	197.35	130.47	123.31	-1899.651	-1699.472	126.817
800	74.047	213.94	139.89	125.05	-1898.156	-1670.992	109.105
900	79.800	228.75	148.95	126.52	-1896.745	-1642.657	95.338
1000	84.537	242.15	157.61	127.81	-1895.432	-1614.512	84.334
1100	88.526	254.39	165.86	128.99	-1894.221	-1586.474	75.336
1200	91.946	265.66	173.71	130.10	-1893.114	-1558.536	67.842
1300	94.922	276.12	181.20	131.15	-1892.109	-1530.709	61.505
1330	95.742	279.12	183.38	131.46	-1891.675	-1523.247	59.825
1330	96.378	279.76	183.38	131.66	-1890.864	-1523.247	59.825
1400	98.143	286.51	188.37	131.66	-1890.373	-1503.007	56.078
1500	100.378	295.59	195.21	131.66	-1889.671	-1475.356	51.377
1600	102.333	304.09	201.76	131.66	-1889.168	-1447.752	47.264
1700	104.058	312.07	208.01	131.66	-1888.858	-1420.194	43.637
1800	105.591	319.59	214.00	131.66	-1921.256	-1392.308	40.404

## MELTING POINT

K

## BOILING POINT

K

## ENTHALPY OF MELTING

kJ

## ENTHALPY OF VAPORIZATION

kJ

 $H_{298}^0 - H_0^0$ 

16.665 kJ

## MOLAR VOLUME

4.4880 J/bar  
44.880 cm<sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

YTTRIUM.... ALPHA-BETA 1752, H. P. 1799 K.

## HEAT CAPACITY EQUATIONS

$$C_p^0 = 1.2106 \times 10^2 + 8.6019 \times 10^{-3} T - 1.8480 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1330 K)

REFERENCE 210

264

264

COMPILED  
5-18-76

YTTERBIUM SESQUIOXIDE (CUBIC)

FORMULA WEIGHT 394.078

$\text{Yb}_2\text{O}_3$ : Alpha crystals 298.15 to 1365 K. Beta crystals 1365 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	133.05	133.05	109.84	-1814.600	-1726.844	302.537
UNCERTAINTY		0.85	0.85		0.850	0.850	0.149
400	30.225	167.87	137.64	122.88	-1812.566	-1697.160	221.627
500	49.238	195.80	146.56	127.16	-1810.425	-1668.560	174.314
600	62.428	219.21	156.78	129.39	-1808.611	-1640.350	142.806
700	72.094	239.26	167.17	130.66	-1806.496	-1612.485	120.326
800	79.465	256.76	177.29	131.41	-1804.504	-1584.909	103.484
900	85.267	272.26	186.99	131.86	-1802.659	-1557.545	90.398
1000	89.939	286.17	196.23	132.13	-1800.978	-1530.418	79.941
1100	93.781	298.77	204.99	132.27	-1818.783	-1503.137	71.378
1200	96.992	310.28	213.29	132.34	-1818.233	-1474.464	64.182
1300	99.711	320.88	221.17	132.34	-1817.735	-1445.857	58.095
1365	101.249	327.39	226.14	132.34	-1851.564	-1344.489	51.450
1365	101.623	327.76	226.14	134.64	-1851.053	-1344.489	51.450
1400	102.450	331.01	228.56	134.64	-1816.717	-1417.143	52.874
1500	104.599	340.30	235.70	134.64	---	---	---
1600	106.476	348.99	242.51	134.64	---	---	---
1700	108.133	357.15	249.02	134.64	---	---	---
1800	109.606	364.84	255.23	134.64	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	19.623 kJ	MOLAR VOLUME	4.2760 J/bar 42.760 $\text{cm}^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

YTTERBIUM.. ALPHA-BETA 1033, M. P. 1097, B. P. 1465 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.3614 \times 10^2 - 2.0174 \times 10^{-3} T - 1.9928 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1365 K)

REFERENCE	207	235	235	COMPILED 8-11-76
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## ZINCITE

FORMULA WEIGHT 81.379

ZnO: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	43.64	43.64	40.62	-350.460	-320.477	56.146
UNCERTAINTY		0.40	0.40		0.270	0.300	0.053
400	11.125	56.45	45.32	45.84	-350.152	-310.274	40.518
500	18.298	66.92	48.62	47.88	-349.665	-300.355	31.378
600	23.335	75.76	52.42	49.10	-349.182	-290.535	25.293
700	27.089	83.41	56.32	50.11	-356.098	-280.722	20.948
800	30.026	90.16	60.13	51.06	-355.843	-269.967	17.627
900	32.411	96.23	63.82	51.99	-355.532	-259.259	15.047
1000	34.419	101.76	67.34	52.91	-355.149	-248.579	12.984
1100	36.141	106.84	70.70	53.81	-354.704	-237.939	11.299
1200	37.648	111.56	73.91	54.65	-469.312	-225.262	9.805
1300	38.987	115.97	76.98	55.44	-467.679	-205.001	8.237
1400	40.186	120.10	79.91	56.15	-465.991	-184.857	6.897
1500	41.273	124.00	82.73	56.77	-464.246	-164.831	5.740
1600	42.257	127.68	85.42	57.29	-462.459	-144.931	4.732
1700	43.154	131.16	88.01	57.70	-460.638	-125.135	3.845
1800	43.971	134.47	90.50	57.99	-458.792	-105.452	3.060

MELTING POINT	2242	K	BOILING POINT		K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION		kJ
$H_{298}^0 - H_0^0$	6.933	kJ	MOLAR VOLUME	1.4338	J/bar cm <sup>3</sup>
				14.338	

## TRANSITIONS IN REFERENCE STATE ELEMENTS

ZINC..... M. P. 692.7, B. P. 1178 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = -13.664 + 4.0569 \times 10^{-2} T - 8.7026 \times 10^{-6} T^2 + 1.1669 \times 10^{-9} T^{-0.5} - 2.1882 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	115	120	41	COMPILED
		215	215	7-29-76

BADDELEYITE

FORMULA WEIGHT 123.219

ZrO<sub>2</sub>: Monoclinic crystals 298.15 to 1478 K. Tetragonal crystals 1478 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	50.38	50.38	56.14	-1100.560	-1042.790	182.693
UNCERTAINTY		0.34	0.34		1.674	1.715	0.300
400	15.350	68.06	52.71	63.68	-1100.141	-1023.113	133.605
500	25.474	82.75	57.28	67.82	-1099.398	-1003.933	104.881
600	32.772	95.37	62.60	70.53	-1098.525	-984.921	85.745
700	38.310	106.39	68.08	72.46	-1097.606	-966.055	72.088
800	42.674	116.17	73.50	73.92	-1096.687	-947.327	61.854
900	46.211	124.94	78.73	75.07	-1095.799	-928.705	53.901
1000	49.146	132.90	83.75	76.01	-1094.958	-910.188	47.544
1100	51.625	140.19	88.57	76.80	-1094.176	-891.754	42.346
1200	53.752	146.90	93.15	77.47	-1097.188	-873.160	38.008
1300	55.598	153.12	97.52	78.05	-1096.137	-854.532	34.336
1400	57.221	158.92	101.70	78.56	-1095.064	-835.994	31.191
1478	58.335	163.18	104.84	78.91	-1094.244	-821.546	29.035
1478	62.387	167.23	104.84	74.48	-1088.254	-821.546	29.035
1500	62.565	168.28	105.72	74.48	-1088.115	-817.552	28.470
1600	63.309	173.10	109.79	74.48	-1087.482	-799.557	26.103
1700	63.966	177.61	113.65	74.48	-1086.873	-781.578	24.015
1800	64.550	181.88	117.33	74.48	-1086.285	-763.658	22.161

MELTING POINT	3123 K	BOILING POINT	K
ENTHALPY OF MELTING	87.027 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	8.749 kJ	MOLAR VOLUME	2.1150 J/bar 21.150 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ZIRCONIUM.. ALPHA-BETA 1136, H. P. 2125 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 90.700 - 4.3877 \times 10^{-2} T^{-0.5} - 8.1334 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1478 K)

REFERENCE	43	264	264	COMPILED
			104	6- 8-76

TIALITE

FORMULA WEIGHT 181.861

Al<sub>2</sub>TiO<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	109.62	109.62	136.40	---	---	---
UNCERTAINTY		0.84	0.84				
400	38.275	153.62	115.34	161.24	---	---	---
500	64.292	191.13	126.84	174.34	---	---	---
600	83.383	223.71	140.33	182.81	---	---	---
700	98.046	252.38	154.33	188.94	---	---	---
800	109.720	277.93	168.21	193.75	---	---	---
900	119.289	300.99	181.70	197.74	---	---	---
1000	127.306	322.01	194.70	201.18	---	---	---
1100	134.164	341.33	207.17	204.24	---	---	---
1200	140.122	359.22	219.10	207.03	---	---	---
1300	145.370	375.90	230.53	209.61	---	---	---
1400	150.043	391.52	241.48	212.04	---	---	---
1500	154.256	406.23	251.97	214.34	---	---	---
1600	158.081	420.13	262.05	216.53	---	---	---
1700	161.582	433.32	271.74	218.65	---	---	---
1800	164.809	445.88	281.07	220.70	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.8750 J/bar 48.750 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.1110 \times 10^2 + 1.4609 \times 10^{-2} T - 6.6101 \times 10^2 T^{-0.5} - 3.6248 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 21 120

COMPILED  
8-2-76



CALCIUM FERRITE

FORMULA WEIGHT 215.772

CaFe<sub>2</sub>O<sub>4</sub>: Crystals 298.15 to melting point 1510 K.

TEMP.						FORMATION FROM THE ELEMENTS GIBBS		
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T	S <sub>T</sub> <sup>o</sup>	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T	C <sub>P</sub> <sup>o</sup>	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>	
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	145.35	145.35	153.64	-1520.340	-1412.666	247.494	
UNCERTAINTY		0.84	0.84		0.120	0.120	0.021	
400	40.650	192.19	151.54	164.03	-1518.063	-1376.217	179.716	
500	65.850	229.36	163.51	168.82	-1515.867	-1340.997	140.094	
600	83.295	260.44	177.14	172.10	-1514.109	-1306.186	113.714	
700	96.189	287.19	191.00	174.97	-1512.943	-1271.685	94.895	
800	106.212	310.73	204.52	177.81	-1513.291	-1237.163	80.779	
900	114.333	331.84	217.51	180.72	-1513.830	-1202.549	69.794	
1000	121.119	351.04	229.92	183.77	-1516.115	-1167.869	61.003	
1100	126.958	368.71	241.75	186.94	-1520.435	-1132.804	53.793	
1200	132.093	385.11	253.02	190.24	-1530.125	-1096.896	47.747	
1300	136.697	400.47	263.77	193.66	-1527.896	-1060.957	42.630	
1400	140.893	414.95	274.06	197.18	-1525.551	-1025.160	38.249	
1500	144.763	428.68	283.92	200.78	-1522.999	-989.467	34.456	

MELTING POINT	1510 K	BOILING POINT	K
ENTHALPY OF MELTING	108.240 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	25.422 kJ	MOLAR VOLUME	4.4980 J/bar 44.980 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

HEAT CAPACITY EQUATION

$$C_P^o = 95.884 + 4.6664 \times 10^{-2} T + 1.4097 \times 10^{-5} T^2 - 3.3600 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1510 K)

REFERENCE	183	214	214	COMPILED
				8- 2-76

## DICALCIUM FERRITE

FORMULA WEIGHT 271.851

Ca<sub>2</sub>Fe<sub>2</sub>O<sub>8</sub>: Crystals 298.15 to melting point 1750 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	188.78	188.78	192.88	-2139.280	-2001.560	350.667
UNCERTAINTY		1.26	1.26		0.850	0.850	0.149
400	52.775	249.52	196.75	217.89	-2136.286	-1954.922	255.288
500	87.012	299.44	212.43	228.74	-2132.584	-1909.984	199.536
600	111.158	341.71	230.55	234.52	-2129.129	-1865.787	162.432
700	129.049	378.14	249.09	238.02	-2126.373	-1822.179	135.973
800	142.826	410.08	267.25	240.38	-2126.140	-1778.672	116.136
900	153.767	438.50	284.73	242.11	-2125.651	-1735.206	100.709
1000	162.670	464.08	301.41	243.49	-2127.487	-1691.751	88.368
1100	170.071	487.34	317.27	244.64	-2131.984	-1647.927	78.254
1200	176.328	508.68	332.35	245.67	-2149.447	-1602.620	69.761
1300	181.698	528.38	346.68	246.61	-2146.520	-1557.251	62.571
1400	186.364	546.69	360.33	247.50	-2143.757	-1512.074	56.416
1500	190.470	563.79	373.32	248.35	-2141.057	-1466.990	51.085
1600	194.113	579.84	385.73	249.18	-2138.511	-1422.161	46.429
1700	197.376	594.98	397.60	250.00	-2138.450	-1377.393	42.322

MELTING POINT	1750 K	BOILING POINT	K
ENTHALPY OF MELTING	151.080 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	31.648 kJ	MOLAR VOLUME	6.7180 J/bar 67.180 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.2228 \times 10^2 + 9.7281 \times 10^{-3} T + 5.4195 \times 10^2 T^{-0.5} - 5.6610 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1750 K)

REFERENCE	183	214	214	COMPILED 8- 2-76
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PEROVSKITE

FORMULA WEIGHT 135.978

CaTiO<sub>3</sub>: Alpha crystals (orthorhombic) 298.15 to 1530 K. Beta crystals (cubic) 1530 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				FORMATION FROM THE ELEMENTS GIBBS		
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>P</sub> <sup>o</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	93.64	93.64	97.65	-1660.630	-1575.256	275.979
UNCERTAINTY		0.42	0.42		1.715	1.757	0.308
400	27.375	125.13	97.76	114.27	-1659.455	-1546.237	201.919
500	45.416	151.33	105.91	119.97	-1657.675	-1518.135	158.599
600	58.082	173.46	115.38	122.60	-1655.926	-1490.389	129.750
700	67.424	192.49	125.07	124.30	-1654.412	-1462.927	109.165
800	74.629	209.19	134.56	125.82	-1653.929	-1435.573	93.734
900	80.400	224.10	143.70	127.42	-1652.923	-1408.330	81.738
1000	85.194	237.62	152.43	129.21	-1652.339	-1381.189	72.146
1100	89.284	250.02	160.74	131.19	-1652.161	-1354.083	64.300
1200	92.865	261.53	168.66	133.38	-1663.354	-1326.208	57.729
1300	96.072	272.30	176.23	135.75	-1661.232	-1298.207	52.163
1400	98.993	282.45	183.46	138.30	-1659.023	-1270.369	47.398
1500	101.705	292.08	190.37	141.00	-1656.689	-1242.674	43.274
1530	102.450	295.28	192.82	141.83	-1655.935	-1234.767	42.155
1530	103.955	296.78	192.82	134.01	-1653.633	-1234.767	42.155
1600	105.264	302.46	197.20	134.01	-1652.602	-1215.442	39.680
1700	106.948	310.58	203.63	134.01	-1651.130	-1188.178	36.508
1800	108.468	318.28	209.81	134.01	-1803.252	-1157.665	33.595

MELTING POINT	2188	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>		kJ	MOLAR VOLUME	3.3626 J/bar 33.626 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.  
 TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

HEAT CAPACITY EQUATION

$$C_P^o = 12.496 + 4.5156 \times 10^{-2} T + 2.4620 \times 10^{-5} T^{2-0.5} - 6.3018 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1530 K)

REFERENCE	177	120	214	COMPILED 7-17-76
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PEROVSKITE FORMULA WEIGHT 135.978

CaTiO<sub>3</sub>: Alpha crystals (orthorhombic) 298.15 to 1530 K. Beta crystals (cubic)  
1530 to 1800 K.

TEMP. K					FORMATION FROM THE OXIDES GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	93.64	93.64	97.65	-80.791 *	-82.323 *	14.423
UNCERTAINTY		0.42	0.42		0.760	0.810	
400	27.375	125.13	97.76	114.27	-80.341 *	-82.901 *	10.826
500	45.416	151.33	105.91	119.97	-79.676 *	-83.616 *	8.735
600	58.082	173.46	115.38	122.60	-79.088 *	-84.458 *	7.353
700	67.424	192.49	125.07	124.30	-78.628 *	-85.397 *	6.372
800	74.629	209.19	134.56	125.82	-78.278 *	-86.390 *	5.641
900	80.400	224.40	143.70	127.42	-78.011 *	-87.425 *	5.074
1000	85.194	237.62	152.43	129.21	-77.772 *	-88.482 *	4.622
1100	89.284	250.02	160.74	131.19	-77.544 *	-89.556 *	4.253
1200	92.865	261.53	168.66	133.38	-77.293 *	-90.661 *	3.946
1300	96.072	272.30	176.23	135.75	-76.989 *	-91.783 *	3.688
1400	98.993	282.45	183.46	138.30	-76.611 *	-92.949 *	3.468
1500	101.705	292.08	190.37	141.00	-76.138 *	-94.123 *	3.278
1530	102.450	295.28	192.82	141.83	-75.931 *	-94.888 *	3.240
1530	103.955	296.78	192.82	134.01	-73.629 *	-94.888 *	3.240
1600	105.264	302.46	197.20	134.01	-73.929 *	-95.609 *	3.121
1700	106.948	310.58	203.63	134.01	-74.358 *	-96.968 *	2.979
1800	108.468	318.28	209.81	134.01	-74.908 *	-98.326 *	2.853

MELTING POINT	2188	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	3.3626 J/bar 33.626 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE OXIDES				

## HEAT CAPACITY EQUATION

$$C_P^0 = 12.496 + 4.5156 \times 10^{-2} T + 2.4620 \times 10^{-5} T^2 - 6.3018 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1530 K)

REFERENCE 177 120 214 COMPILED 7-17-76

COBALT SPINEL

FORMULA WEIGHT 240.797

Co<sub>3</sub>O<sub>4</sub>: Crystals 298.15 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	102.51	102.51	123.05	-891.190	-772.553	135.349
UNCERTAINTY		0.84	0.84		8.500	8.500	1.489
400	34.725	142.43	107.71	144.84	-891.199	-731.979	95.587
500	57.598	175.67	118.07	152.84	-890.632	-692.247	72.319
600	74.093	204.19	130.10	160.63	-889.991	-652.613	56.815
700	87.153	229.69	142.54	170.88	-889.067	-613.134	45.753
800	98.404	253.33	154.93	183.92	-888.845	-573.621	37.454
900	108.744	275.86	167.12	199.49	-886.561	-534.328	31.012
1000	118.692	297.78	179.09	217.25	-883.346	-495.366	25.875

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.9770 J/bar 39.770 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

COBALT..... ALPHA-BETA 700, CURIE P. 1394, M. P. BETA 1768 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -4.8355 \times 10^2 + 0.34236 T + 1.1845 \times 10^{-4} T^{-0.5} - 1.6129 \times 10^{-7} T^{-2}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	129	263	263	COMPILED 8- 4-76
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## CHROMITE

FORMULA WEIGHT 223.837

FeCr<sub>2</sub>O<sub>4</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	146.02	146.02	133.64	---	---	---
UNCERTAINTY		1.67	1.67				
400	36.275	187.75	151.48	149.96	---	---	---
500	60.126	222.43	162.30	160.53	---	---	---
600	77.515	252.39	174.88	167.96	---	---	---
700	90.844	278.71	187.87	173.42	---	---	---
800	101.439	302.15	200.71	177.60	---	---	---
900	110.089	323.27	213.18	180.90	---	---	---
1000	117.311	342.47	225.16	183.60	---	---	---
1100	123.445	360.08	236.64	185.89	---	---	---
1200	128.734	376.35	247.62	187.90	---	---	---
1300	133.357	391.46	258.10	189.74	---	---	---
1400	137.450	405.59	268.14	191.47	---	---	---
1500	141.104	418.85	277.75	193.14	---	---	---
1600	144.409	431.37	286.96	194.81	---	---	---
1700	147.424	443.23	295.81	196.51	---	---	---
1800	150.199	454.51	304.31	198.27	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.4010 J/bar 44.010 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.  
CHROMIUM... M. P. 2130 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 3.0184 \times 10^2 - 4.1571 \times 10^{-2} T + 1.1470 \times 10^{-5} T^2 - 2.8027 \times 10^3 T^{-0.5} \\ + 4.8769 \times 10^5 T^{-2} \\ \text{(EQUATION VALID FROM 298 - 1800 K)}$$

REFERENCE 174 120

COMPILED  
7-17-76

ILMENITE

FORMULA WEIGHT 151.745

FeTiO<sub>3</sub>: Crystals 298.15 to melting point 1640 K. Liquid 1640 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	105.86	105.86	99.50	-1236.622	-1159.170	203.083
UNCERTAINTY		1.25	1.25		1.590	1.632	0.286
400	27.275	137.25	109.97	112.45	-1235.523	-1132.854	147.936
500	44.886	162.96	118.07	117.63	-1234.099	-1107.341	115.684
600	57.297	184.71	127.41	120.92	-1232.752	-1082.114	94.207
700	66.594	203.57	136.98	123.84	-1231.587	-1057.125	78.884
800	73.938	220.30	146.36	126.87	-1230.674	-1032.266	67.400
900	80.000	235.43	155.43	130.14	-1230.104	-1007.463	58.472
1000	85.187	249.33	164.14	133.69	-1230.137	-982.744	51.333
1100	89.767	262.24	172.47	137.51	-1230.896	-957.935	45.489
1200	93.913	274.38	180.47	141.57	-1234.603	-933.023	40.614
1300	97.743	285.88	188.14	145.85	-1232.068	-908.028	36.485
1400	101.336	296.85	195.51	150.33	-1229.337	-883.221	32.954
1500	104.758	307.38	202.62	154.97	-1226.333	-858.572	29.898
1600	105.541	314.68	209.14	159.76	-1227.093	-833.623	27.215
1640	106.523	318.57	212.05	161.71	-1226.352	-824.285	26.254
1640	161.808	373.85	212.05	199.16	-1135.684	-824.285	26.254
1700	163.126	380.71	217.58	199.16	-1132.527	-812.407	24.962
1800	165.128	392.13	227.00	199.16	-1125.878	-793.789	23.035

MELTING POINT	1640 K	BOILING POINT	K
ENTHALPY OF MELTING	90.667 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	3.1690 J/bar 31.690 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.  
TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -2.9895 + 6.5049 \times 10^{-2} T + 2.4266 \times 10^{-5} T^2 - 5.1057 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1640 K)

REFERENCE	177	120	122	COMPILED 7-17-76
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## ILMENITE

FORMULA WEIGHT 151.745

FeTiO<sub>3</sub>: Crystals 298.15 to melting point 1640 K. Liquid 1640 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	105.86	105.86	99.50	-19.829 *	-18.568 *	3.253
UNCERTAINTY		1.25	1.25		2.300	2.340	
400	27.275	137.25	109.97	112.45	-20.049 *	-18.093 *	2.363
500	44.886	162.96	118.07	117.63	-20.074 *	-17.599 *	1.839
600	57.297	184.71	127.41	120.92	-20.134 *	-17.092 *	1.488
700	66.594	203.57	136.98	123.84	-20.239 *	-16.585 *	1.238
800	73.938	220.30	146.36	126.87	-20.343 *	-16.055 *	1.048
900	80.000	235.43	155.43	130.14	-20.399 *	-15.512 *	0.900
1000	85.187	249.33	164.14	133.69	-20.350 *	-14.980 *	0.782
1100	89.767	262.24	172.47	137.51	-20.161 *	-14.441 *	0.686
1200	93.913	274.38	180.47	141.57	-19.792 *	-13.936 *	0.607
1300	97.743	285.88	188.14	145.85	-19.209 *	-13.463 *	0.541
1400	101.336	296.85	195.51	150.33	-18.389 *	-13.055 *	0.487
1500	104.758	307.38	202.62	154.97	-17.303 *	-12.713 *	0.443
1600	105.541	314.68	209.14	159.76	-19.940 *	-11.897 *	0.388
1640	106.523	318.57	212.05	161.71	-19.921 *	-10.548 *	0.336
1640	161.808	373.85	212.05	199.16	70.747 *	-10.548 *	0.336
1700	163.126	380.71	217.58	199.16	51.595 *	-12.014 *	0.369
1800	165.128	392.13	227.00	199.16	56.450 *	-15.980 *	0.464

MELTING POINT	1640	K	BOILING POINT		K
ENTHALPY OF MELTING	90.667	kJ	ENTHALPY OF VAPORIZATION		kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	3.1690	J/bar cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

FeO..... M. P. 1650 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -2.9895 + 6.5049 \times 10^{-2} T + 2.4266 \times 10^{-5} T^2 - 5.1057 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1640 K)

REFERENCE	177	120	122	COMPILED 7-17-76
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TITANOHAZMETHITE

FORMULA WEIGHT 223.592

Fe<sub>2</sub>TiO<sub>4</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>P</sub> <sup>o</sup> J/mol·K			
298.15	0.000	168.87	168.87	142.30	---	---	---
UNCERTAINTY		2.51	2.51				
400	39.050	213.81	174.76	160.82	---	---	---
500	64.178	250.53	186.35	167.82	---	---	---
600	81.868	281.57	199.70	172.72	---	---	---
700	95.199	308.56	213.36	177.75	---	---	---
800	105.869	332.66	226.79	183.51	---	---	---
900	114.856	354.65	239.79	190.10	---	---	---
1000	122.741	375.05	252.31	197.48	---	---	---
1100	129.897	394.25	264.35	205.56	---	---	---
1200	136.561	412.51	275.95	214.26	---	---	---
1300	142.889	430.02	287.13	223.48	---	---	---
1400	148.986	446.93	297.94	233.16	---	---	---
1500	154.933	463.36	308.43	243.23	---	---	---
1600	160.776	479.39	318.61	253.66	---	---	---
1700	166.554	495.08	328.53	264.38	---	---	---
1800	172.293	510.50	338.21	275.38	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	kJ	MOLAR VOLUME	4.6820 J/bar 46.820 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.  
TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

HEAT CAPACITY EQUATION

$$C_P^o = - 1.0257 \times 10^{-2} + 0.14252 T + 5.2707 \times 10^{-3} T^{-0.5} - 9.1445 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 21 120 COMPILED 8- 2-76

## PSEUDOBROOKITE

FORMULA WEIGHT 239.591

Fe<sub>2</sub>TiO<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	156.48	156.48	164.26	---	---	---
UNCERTAINTY		1.25	1.25				
400	44.275	207.44	163.16	181.43	---	---	---
500	72.714	249.02	176.31	190.86	---	---	---
600	92.963	284.41	191.45	197.22	---	---	---
700	108.214	315.19	206.98	202.02	---	---	---
800	120.192	342.43	222.24	205.94	---	---	---
900	129.911	366.89	236.98	209.30	---	---	---
1000	138.002	389.10	251.10	212.30	---	---	---
1100	144.883	409.46	264.58	215.04	---	---	---
1200	150.836	428.28	277.44	217.58	---	---	---
1300	156.064	445.79	289.73	219.99	---	---	---
1400	160.714	462.18	301.47	222.29	---	---	---
1500	164.893	477.59	312.70	224.51	---	---	---
1600	168.686	492.15	323.46	226.65	---	---	---
1700	172.157	505.96	333.80	228.74	---	---	---
1800	175.357	519.09	343.73	230.78	---	---	---

## MELTING POINT

K

## BOILING POINT

K

## ENTHALPY OF MELTING

kJ

## ENTHALPY OF VAPORIZATION

kJ

 $H_{298}^0 - H_0^0$ 

kJ

## MOLAR VOLUME

5.4530 J/bar  
54.530 cm<sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.1356 \times 10^2 + 1.6245 \times 10^{-2} T - 4.7946 \times 10^2 T^{-0.5} - 2.3447 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 21 120

COMPILED  
8- 2-76

LITHIUM ALUMINATE (ALPHA) FORMULA WEIGHT 65.921

$\text{LiAlO}_2$ : Crystals 298.15 to melting point 1883 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	53.35	53.35	67.81	-1188.670	-1126.276	197.320
UNCERTAINTY		2.10	2.10		4.180	4.180	0.732
400	19.225	75.44	56.21	81.39	-1189.215	-1104.851	144.279
500	32.400	94.40	62.00	88.25	-1192.306	-1083.441	113.187
600	42.092	110.90	68.81	92.57	-1192.119	-1061.685	92.428
700	49.534	125.41	75.88	95.68	-1191.740	-1039.973	77.604
800	55.461	138.35	82.89	98.13	-1191.282	-1018.314	66.489
900	60.322	150.03	89.71	100.20	-1190.822	-996.719	57.848
1000	64.400	160.69	96.29	102.02	-1201.065	-974.425	50.899
1100	67.897	170.49	102.59	103.68	-1200.336	-951.780	45.196
1200	70.944	179.58	108.64	105.23	-1199.491	-929.227	40.448
1300	73.638	188.06	114.42	106.69	-1198.530	-906.732	36.433
1400	76.050	196.02	119.97	108.10	-1197.461	-884.337	32.995
1500	78.233	203.52	125.29	109.46	-1196.279	-862.004	30.018
1600	80.226	210.63	130.40	110.79	-1194.988	-839.772	27.416
1700	82.063	217.39	135.33	112.09	-1338.844	-809.787	24.882
1800	83.767	223.83	140.06	113.37	-1336.550	-778.712	22.598

MELTING POINT	1883 K	BOILING POINT	K
ENTHALPY OF MELTING	87.900 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.5210 J/bar 25.210 $\text{cm}^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

LITHIUM... M. P. 453.69, B. P. 1618 K.

ALUMINUM... M. P. 933 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 95.382 + 1.1387 \times 10^{-2} T - 75.392 T^{-0.5} - 2.3647 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	32	32	32	COMPILED 5-19-76
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## SPINEL

FORMULA WEIGHT 142.267

MgAl<sub>2</sub>O<sub>4</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>p</sub> <sup>0</sup> J/mol·K			
298.15	0.000	80.63	80.63	115.94	-2299.320	-2174.860	381.028
UNCERTAINTY		0.42	0.42		0.750	0.760	0.133
400	32.500	118.00	85.50	137.27	-2300.065	-2131.541	278.352
500	54.806	150.08	95.27	149.86	-2299.704	-2089.439	218.283
600	71.415	178.21	106.80	158.58	-2298.833	-2047.457	178.248
700	84.354	203.17	118.82	165.13	-2297.757	-2005.654	149.664
800	94.787	225.57	130.78	170.33	-2296.663	-1963.991	128.236
900	103.433	245.89	142.46	174.64	-2295.686	-1922.456	111.577
1000	110.737	264.49	153.75	178.30	-2325.192	-1878.752	98.136
1100	117.027	281.63	164.60	181.49	-2323.824	-1834.159	87.097
1200	122.519	297.55	175.03	184.31	-2322.247	-1789.723	77.905
1300	127.372	312.40	185.03	186.85	-2320.474	-1745.393	70.131
1400	131.707	326.34	194.63	189.17	-2445.485	-1697.647	63.340
1500	135.608	339.46	203.85	191.30	-2442.192	-1644.342	57.261
1600	139.151	351.87	212.72	193.27	-2438.746	-1591.258	51.949
1700	142.390	363.64	221.25	195.12	-2435.154	-1538.421	47.270
1800	145.368	374.85	229.48	196.86	-2431.428	-1485.780	43.116

MELTING POINT	2408	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	15.410	kJ	MOLAR VOLUME	3.9710 J/bar 39.710 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

ALUMINUM... M. P. 933 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 2.2291 \times 10^2 + 6.1267 \times 10^{-3} T - 1.5512 \times 10^{-5} T^2 + 1.6857 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	22	214	237	COMPILED
			31	8- 2-76

PICROCHROMITE

FORMULA WEIGHT 192.295

MgCr<sub>2</sub>O<sub>4</sub>: Crystals 298.15 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	106.02	106.02	126.78	-1783.640	-1669.079	292.417
UNCERTAINTY		0.84	0.84		8.370	8.400	1.472
400	35.325	146.63	111.30	147.92	-1783.163	-1629.971	212.853
500	59.018	180.91	121.89	158.75	-1781.786	-1591.836	166.299
600	76.242	210.49	134.25	165.51	-1780.051	-1553.995	135.288
700	89.350	236.38	147.03	170.22	-1778.236	-1516.464	113.160
800	99.690	259.35	159.66	173.76	-1776.495	-1479.199	96.582
900	108.078	279.99	171.91	176.58	-1774.932	-1442.112	83.698
1000	115.051	298.72	183.67	178.90	-1782.554	-1404.444	73.361
1100	120.949	315.86	194.91	180.89	-1781.414	-1366.692	64.899
1200	126.019	331.68	205.66	182.64	-1780.499	-1329.035	57.852
1300	130.435	346.36	215.92	184.20	-1779.835	-1291.438	51.891
1400	134.329	360.06	225.73	185.62	-1906.419	-1250.281	46.649
1500	137.791	372.92	235.13	186.92	-1905.172	-1203.472	41.909
1600	140.899	385.02	244.12	188.13	-1904.263	-1156.727	37.763
1700	143.712	396.46	252.75	189.27	-1903.712	-1110.033	34.107
1800	146.274	407.31	261.04	190.35	-1903.544	-1063.376	30.859

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	4.3560 J/bar 43.560 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

CHROMIUM... M. P. 2130 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.9614 \times 10^2 + 5.3977 \times 10^{-3} T - 6.1688 \times 10^2 T^{-0.5} - 3.1260 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	174	214	214	COMPILED 7-17-76
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## PICROCHROMITE

FORMULA WEIGHT 192.295

HgCr<sub>2</sub>O<sub>6</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	106.02	106.02	126.78	-47.450 *	-46.827 *	8.204
UNCERTAINTY		0.84	0.84		8.370	8.400	
400	35.325	146.63	111.30	147.92	-48.620 *	-46.492 *	6.071
500	59.018	180.91	121.89	158.75	-49.312 *	-45.872 *	4.792
600	76.242	210.49	134.25	165.51	-49.666 *	-45.142 *	3.930
700	89.350	236.38	147.03	170.22	-49.812 *	-44.373 *	3.311
800	99.690	259.35	159.66	173.76	-49.841 *	-43.601 *	2.847
900	108.078	279.99	171.91	176.58	-49.810 *	-42.826 *	2.486
1000	115.051	298.72	183.67	178.90	-49.744 *	-42.054 *	2.197
1100	120.949	315.86	194.91	180.89	-49.664 *	-41.282 *	1.960
1200	126.019	331.68	205.66	182.64	-49.577 *	-40.529 *	1.764
1300	130.435	346.36	215.92	184.20	-49.487 *	-39.776 *	1.598
1400	134.329	360.06	225.73	185.62	-49.390 *	-39.016 *	1.456
1500	137.791	372.92	235.13	186.92	-49.283 *	-38.303 *	1.334
1600	140.899	385.02	244.12	188.13	-49.162 *	-37.578 *	1.227
1700	143.712	396.46	252.75	189.27	-49.016 *	-36.844 *	1.132
1800	146.274	407.31	261.04	190.35	-48.842 *	-36.152 *	1.049

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	KJ	MOLAR VOLUME	4.3560 J/bar 43.560 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.9614 \times 10^2 + 5.3977 \times 10^{-3} T - 6.1688 \times 10^2 T^{-0.5} - 3.1260 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	174	214	214	COMPILED 7-17-76
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MAGNESIOFERRITE

FORMULA WEIGHT 199.997

HgFe<sub>2</sub>O<sub>4</sub>: Alpha crystals 298.15 to 665 K. Beta crystals 665 to 1230 K.  
Gamma crystals 1230 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	123.85	123.85	143.72	-1428.420	-1317.004	230.735
UNCERTAINTY		0.84	0.84		1.841	1.883	0.330
400	39.350	169.11	129.76	164.30	-1426.641	-1279.171	167.043
500	66.022	207.59	141.57	180.83	-1423.820	-1242.595	129.814
600	86.428	241.91	155.48	196.01	-1420.197	-1206.670	105.050
665	97.601	262.55	164.95	205.88	-1418.140	-1185.187	93.095
665	97.601	262.55	164.59	186.68	-1418.140	-1185.187	93.095
700	102.857	272.03	169.17	187.13	-1416.079	-1170.817	87.368
800	113.470	297.10	183.63	188.40	-1414.267	-1135.915	74.168
900	121.867	319.36	197.49	189.68	-1413.500	-1101.103	63.907
1000	128.711	339.41	210.70	190.95	-1423.296	-1065.610	55.662
1100	134.426	357.67	223.24	192.23	-1425.959	-1029.671	48.895
1200	139.296	374.45	235.15	193.50	-1426.829	-993.684	43.254
1230	140.623	379.23	238.61	193.88	-1426.207	-982.951	41.743
1230	141.592	380.20	238.61	176.92	-1425.015	-982.951	41.743
1300	143.602	390.10	246.50	180.93	-1424.600	-957.768	38.484
1400	146.471	403.72	257.25	186.64	-1550.717	-918.344	34.264
1500	149.340	416.79	267.45	192.36	-1548.260	-873.195	30.407
1600	152.207	429.39	277.18	198.07	-1545.451	-828.308	27.042
1700	155.073	441.57	286.50	203.79	-1544.627	-783.525	24.075
1800	157.938	453.38	295.44	209.50	-1541.769	-738.786	21.439

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	4.4570 J/bar 44.570 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.7820 \times 10^{-2} + 1.2752 \times 10^{-5} T$$

(EQUATION VALID FROM 665 - 1230 K)

$$C_P^0 = 1.0662 \times 10^{-2} + 5.7158 \times 10^{-5} T$$

(EQUATION VALID FROM 1230 - 1800 K)

REFERENCE	183	120	214	COMPILED
			146	8- 2-76

## GEIKELITE

FORMULA WEIGHT 120.203

HgTiO<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	74.56	74.56	91.76	-1572.765	-1484.371	260.057	
UNCERTAINTY		0.42	0.42		1.590	1.630	0.285	
400	25.725	104.13	78.40	107.77	-1572.228	-1454.218	189.902	
500	42.910	129.02	86.11	114.78	-1571.022	-1424.857	148.854	
600	55.255	150.34	95.09	118.89	-1569.645	-1395.750	121.511	
700	64.564	168.89	104.33	121.83	-1568.273	-1366.876	101.998	
800	71.877	185.33	113.45	124.26	-1566.967	-1338.203	87.376	
900	77.822	200.09	122.27	126.47	-1565.748	-1309.662	76.011	
1000	82.793	213.52	130.73	128.56	-1573.568	-1280.508	66.887	
1100	87.046	225.87	138.82	130.60	-1572.416	-1251.260	59.418	
1200	90.759	237.32	146.56	132.60	-1575.283	-1221.961	53.191	
1300	94.055	248.02	153.97	134.59	-1573.590	-1192.599	47.919	
1400	97.021	258.06	161.04	136.56	-1698.814	-1159.744	43.271	
1500	99.721	267.55	167.83	138.50	-1695.847	-1121.347	39.049	
1600	102.206	276.55	174.34	140.43	-1692.827	-1083.139	35.361	
1700	104.510	285.12	180.61	142.33	-1689.756	-1045.142	32.113	
1800	106.663	293.31	186.65	144.20	-1686.633	-1007.313	29.232	

MELTING POINT	1903	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	13.556	kJ	MOLAR VOLUME	3.0860 J/bar 30.860 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 61.635 + 3.7673 \times 10^{-2} T - 3.5882 \times 10^{-6} T^2 + 1.1759 \times 10^{-9} T^3 - 4.3444 \times 10^{-12} T^4$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	177	120	214	COMPILED 7-17-76
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GEIKELITE

FORMULA WEIGHT 120.203

MgTiO<sub>3</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	74.56	74.56	91.76	-26.525 *	-25.729 *	4.508
UNCERTAINTY		0.42	0.42		0.920	0.960	
400	25.725	104.13	78.40	107.77	-26.285 *	-25.481 *	3.327
500	42.910	129.02	86.11	114.78	-25.826 *	-25.331 *	2.646
600	55.255	150.34	95.09	118.89	-25.345 *	-25.279 *	2.201
700	64.564	168.89	104.33	121.83	-24.888 *	-25.301 *	1.888
800	71.877	185.33	113.45	124.26	-24.460 *	-25.404 *	1.659
900	77.822	200.09	122.27	126.47	-24.055 *	-25.540 *	1.482
1000	82.793	213.52	130.73	128.56	-23.646 *	-25.716 *	1.343
1100	87.046	225.87	138.82	130.60	-23.233 *	-25.950 *	1.232
1200	90.759	237.32	146.56	132.60	-22.798 *	-26.218 *	1.141
1300	94.055	248.02	153.97	134.59	-22.329 *	-26.528 *	1.066
1400	97.021	258.06	161.04	136.56	-21.815 *	-26.855 *	1.002
1500	99.721	267.55	167.83	138.50	-21.250 *	-27.250 *	0.949
1600	102.206	276.55	174.34	140.43	-20.622 *	-27.662 *	0.903
1700	104.510	285.12	180.61	142.33	-19.924 *	-28.118 *	0.864
1800	106.663	293.31	186.65	144.20	-19.152 *	-28.638 *	0.831

MELTING POINT	1903	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	13.556	kJ	MOLAR VOLUME	3.0860 J/bar 30.860 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

HEAT CAPACITY EQUATION

$$C_P^0 = 61.635 + 3.7673 \times 10^{-2} T - 3.5882 \times 10^{-6} T^2 + 1.1759 \times 10^{-9} T^3 - 4.3444 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE 177 120 214 COMPILED 7-17-76

## ZINC TITANIUM SPINEL

FORMULA WEIGHT 242.658

Zn<sub>2</sub>TiO<sub>4</sub>: Crystals 298.15 to 1800 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	143.09	143.09	133.58	-1647.660	-1534.035	268.758
UNCERTAINTY		0.28	0.28		2.510	2.510	0.440
400	36.525	185.12	148.59	151.79	-1646.976	-1495.288	195.265
500	60.804	220.31	159.51	163.31	-1645.361	-1457.541	152.269
600	78.605	250.84	172.24	171.48	-1643.290	-1420.156	123.636
700	92.333	277.76	185.43	177.63	-1655.715	-1382.995	103.201
800	103.307	301.80	198.49	182.44	-1653.625	-1344.169	87.766
900	112.322	323.52	211.20	186.30	-1651.336	-1305.619	75.776
1000	119.884	343.32	223.44	189.47	-1648.912	-1267.332	66.199
1100	126.334	361.51	235.18	192.12	-1646.401	-1229.303	58.375
1200	131.912	378.32	246.41	194.35	-1878.124	-1187.164	51.676
1300	136.790	393.96	257.17	196.25	-1872.947	-1129.815	45.397
1400	141.100	408.56	267.46	197.89	-1867.759	-1072.839	40.028
1500	144.932	422.27	277.34	199.30	-1862.590	-1016.230	35.388
1600	148.369	435.17	286.80	200.53	-1857.441	-959.985	31.340
1700	151.470	447.36	295.89	201.60	-1852.329	-904.069	27.779
1800	154.281	458.91	304.63	202.53	-1847.266	-848.410	24.620

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.5580 J/bar 45.580 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

ZINC..... M. P. 692.7, B. P. 1178 K.

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.6129 \times 10^2 - 5.1374 \times 10^{-3} T - 2.0949 \times 10^{-5} T^{-0.5} - 4.3165 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	21	264	264	COMPILED 8- 2-76
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BRONARGYRITE

FORMULA WEIGHT 187.772

AgBr: Crystals 298.15 to melting point 703 K. Liquid 703 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	107.11	107.11	52.38	-100.580	-97.121	17.015
UNCERTAINTY		0.42	0.42		0.180	0.180	0.032
400	14.175	123.42	109.24	58.94	-114.829	-92.932	12.136
500	23.772	137.26	113.49	65.39	-113.070	-87.650	9.157
600	31.243	149.76	118.52	71.83	-110.727	-82.780	7.207
700	37.501	161.31	123.81	78.27	-107.810	-78.342	5.846
703	37.700	162.63	124.93	78.47	-107.621	-78.387	5.824
703	50.734	175.66	124.93	62.34	-98.458	-78.387	5.824
800	52.142	182.76	130.62	62.34	-97.009	-75.515	4.931
900	53.277	190.08	136.80	62.34	-95.516	-72.888	4.230
1000	54.183	196.65	142.46	62.34	-94.109	-70.450	3.680

MELTING POINT	703	K	BOILING POINT	K
ENTHALPY OF MELTING	9.163	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	2.8991 J/bar 28.991 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILVER..... M. P. 1234 K.

BROMINE.... B. P. 332 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 33.169 + 6.4434 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 703 K)

REFERENCE	115	120	215	COMPILED
		215		6- 2-76

## POTASSIUM BROMIDE

FORMULA WEIGHT 119.002

KBr: Crystals 298.15 to melting point 1007 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	95.90	95.90	52.30	-393.460	-380.061	66.585
UNCERTAINTY		0.20	0.20		0.180	0.180	0.032
400	13.550	111.54	97.99	53.87	-410.879	-371.930	48.569
500	21.710	123.65	101.94	54.79	-410.401	-362.236	37.843
600	27.333	133.76	106.43	56.20	-409.751	-352.668	30.703
700	31.594	142.57	110.98	58.21	-408.897	-343.218	25.611
800	35.075	150.50	115.42	60.75	-407.806	-333.904	21.802
900	38.089	157.83	119.74	63.74	-406.454	-324.750	18.848
1000	40.821	164.71	123.89	67.09	-404.813	-315.746	16.493

MELTING POINT	1007 K	BOILING POINT	1671 K
ENTHALPY OF MELTING	25.500 kJ	ENTHALPY OF VAPORIZATION	149.200 kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.3280 J/bar 43.280 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

BROMINE.... B. P. 332 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = -43.924 + 5.8546 \times 10^{-2} T + 1.7173 \times 10^{-5} T^{-0.5} - 1.8391 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	247	215	215	COMPILED
	173			6-29-76

STRONTIUM BROMIDE

FORMULA WEIGHT 247.428

SrBr<sub>2</sub>: Crystals 298.15 to 900 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	135.10	135.10	75.35	-717.560	-695.908	121.921
UNCERTAINTY		0.20	0.20		0.850	0.850	0.149
400	19.875	158.01	138.14	79.69	-747.032	-682.375	89.109
500	32.016	175.98	143.96	81.44	-745.595	-666.379	69.616
600	40.433	191.02	150.59	83.76	-744.162	-650.667	56.646
700	46.853	204.17	157.32	87.15	-742.670	-635.204	47.400
800	52.157	216.09	163.93	91.58	-741.039	-619.962	40.480
900	56.822	227.18	170.36	96.89	-739.886	-604.873	35.106

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	17.828 kJ	MOLAR VOLUME	5.8310 J/bar 58.310 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

STRONTIUM.. ALPHA-GAMMA 828, M. P. GAMMA 1041, B. P. 1652 K.

BROMINE.... B. P. 332 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -1.2317 \times 10^2 + 0.11349 T + 3.7012 \times 10^3 T^{-0.5} - 4.4156 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	250	250	214	COMPILED 7- 1-76
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## TITANIUM TRIBROMIDE

FORMULA WEIGHT 287.612

TiBr<sub>3</sub>: Crystals 298.15 to 1200 K.

TEMP.	FORMATION FROM THE ELEMENTS						Log K <sub>f</sub>
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	GIBBS FREE ENERGY	
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	176.44	176.44	101.71	-595.380	-570.732	99.990
UNCERTAINTY		3.35	3.35		8.370	8.450	1.480
400	25.750	206.15	180.40	103.80	-639.619	-553.109	72.229
500	42.452	230.48	188.03	115.17	-636.924	-531.779	55.555
600	55.590	252.55	196.96	127.27	-633.157	-511.080	44.494
700	66.630	273.02	206.39	138.23	-628.359	-491.104	36.647
800	76.189	292.11	215.92	147.71	-622.655	-471.876	30.810
900	84.600	309.99	225.39	155.81	-616.183	-453.404	26.315
1000	92.072	326.77	234.70	162.68	-609.082	-435.692	22.758
1100	98.764	342.56	243.80	168.51	-601.459	-418.726	19.884
1200	104.788	357.44	252.65	173.46	-597.458	-402.309	17.512

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	6.7800 J/bar 67.800 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

BROMINE.... B. P. 332 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 3.9749 \times 10^2 - 2.6092 \times 10^{-2} T - 6.9169 \times 10^3 T^{-0.5} + 1.0014 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	141	247	247	COMPILED
				6- 2-76

CHLORARGYRITE

FORMULA WEIGHT 143.321

AgCl: Crystals 298.15 to melting point 728 K. Liquid 728 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	96.23	96.23	50.79	-127.070	-109.819	19.240
UNCERTAINTY		0.20	0.20		0.085	0.085	0.015
400	13.775	112.08	98.30	56.65	-125.938	-104.086	13.592
500	22.678	125.08	102.40	59.70	-124.502	-98.787	10.320
600	29.025	136.15	107.13	61.70	-122.900	-93.789	8.165
700	33.806	145.78	111.97	63.21	-121.208	-89.071	6.647
728	34.932	148.97	114.04	63.81	-120.678	-88.257	6.333
728	52.634	166.67	114.04	66.94	-107.791	-88.257	6.333
800	53.921	172.34	118.42	66.94	-106.373	-85.939	5.611
900	55.368	180.20	124.84	66.94	-104.404	-83.482	4.845
1000	52.342	187.27	134.93	66.94	-106.706	-85.460	4.464

MELTING POINT	728	K	BOILING POINT	K
ENTHALPY OF MELTING	12.887	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	12.033	kJ	MOLAR VOLUME	2.5727 J/bar 25.727 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SILVER..... H. P. 1234 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 59.955 + 7.6201 \times 10^{-3} T - 1.0167 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 728 K)

REFERENCE	115	120	215	COMPILED
		215		7- 1-76

## HYDROPHILITE

FORMULA WEIGHT 110.986

CaCl<sub>2</sub>: Crystals 298.15 to melting point 1055 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	104.60	104.60	72.59	-795.800	-748.063	131.058
UNCERTAINTY		1.25	1.25		0.650	0.750	0.131
400	18.975	126.47	107.49	75.90	-794.363	-731.971	95.586
500	30.528	143.59	113.06	77.48	-792.949	-716.539	74.857
600	38.453	157.82	119.37	78.64	-791.629	-701.377	61.061
700	44.273	170.03	125.76	79.73	-790.450	-686.437	51.223
800	48.774	180.75	131.98	80.85	-790.165	-671.565	43.849
900	52.400	190.34	137.94	82.06	-789.218	-656.801	38.120
1000	55.434	199.05	143.62	83.37	-788.567	-642.117	33.541

MELTING POINT	1055	K	BOILING POINT	K
ENTHALPY OF MELTING	28.368	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	5.0750 J/bar 50.750 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS				

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 76.846 + 6.6490 \times 10^{-6} T^2 - 1.2847 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1055 K)

REFERENCE	115	214	214	COMPILED
	169			6-14-76



LAURENCITE

FORMULA WEIGHT 126.753

FeCl<sub>2</sub>: Crystals 298.15 to melting point 950 K. Liquid 950 to boiling point 1347 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	117.95	117.95	76.32	-341.650	-302.172	52.939
UNCERTAINTY		0.42	0.42		0.420	0.420	0.074
400	20.225	141.26	121.03	81.01	-339.749	-288.974	37.736
500	32.446	159.41	126.96	81.47	-338.007	-276.474	28.883
600	40.643	174.29	133.65	81.90	-336.528	-264.307	23.010
700	46.616	186.99	140.37	83.15	-335.262	-252.388	18.833
800	51.307	198.23	146.92	85.29	-334.188	-240.632	15.712
900	55.244	208.44	153.20	88.26	-333.337	-228.965	13.289
950	56.902	213.51	156.61	90.01	-332.832	-223.522	12.290
950	102.177	258.79	156.61	102.17	-289.820	-223.522	12.290
1000	102.173	263.64	161.47	102.17	-289.477	-219.664	11.474
1100	102.165	273.34	171.17	102.17	-288.791	-212.654	10.098
1200	102.159	282.21	180.05	102.17	-287.239	-205.828	8.959
1300	102.154	290.41	188.26	102.17	-284.230	-199.233	8.005

MELTING POINT	950 K	BOILING POINT	1347 K
ENTHALPY OF MELTING	43.012 kJ	ENTHALPY OF VAPORIZATION	124.809 kJ
$H_{298}^0 - H_0^0$	16.272 kJ	MOLAR VOLUME	3.9460 J/bar 39.460 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -1.1231 \times 10^{-2} + 8.9510 \times 10^{-2} T + 3.7897 \times 10^{-5} T^{-0.5} - 5.1145 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 950 K)

REFERENCE	169	215	215 147	COMPILED 7- 1-76
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## MOLYSITE

FORMULA WEIGHT 162.206

FeCl<sub>3</sub>: Crystals 298.15 to melting point 577 K. Liquid 577 to boiling point 605 K. Ideal gas (dimer) 605 to 700 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	142.26	142.26	94.93	-399.240	-333.754	58.473
UNCERTAINTY		0.42	0.42		0.420	1.420	0.249
400	25.887	172.05	146.16	123.68	-396.840	-311.729	40.708
500	43.220	197.11	153.89	123.68	-393.759	-290.773	30.377
577	46.367	207.97	161.60	123.68	-395.087	-275.554	24.945
577	121.055	282.66	161.60	133.89	-351.992	-275.554	24.945
600	128.352	294.22	165.87	133.89	-346.857	-272.244	23.701
605	128.397	295.23	166.82	133.89	-346.647	-271.885	23.474
605	164.566	331.38	166.82	71.13	-324.764	-271.885	23.474
700	154.503	344.51	190.01	71.13	-324.532	-263.199	19.640

MELTING POINT	577 K	BOILING POINT	605 K
ENTHALPY OF MELTING	43.095 kJ	ENTHALPY OF VAPORIZATION	21.882 kJ
$H_{298}^0 - H_0^0$	19.707 kJ	MOLAR VOLUME	5.7860 J/bar 57.860 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.2368 \times 10^2 - 2.5564 \times 10^2 T^{-2}$$

(EQUATION VALID FROM 298 - 577 K)

REFERENCE	169	215	215	COMPILED
			147	7-24-76

HYDROGEN CHLORIDE

FORMULA WEIGHT 36.461

HCl: Ideal gas 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	186.90	186.90	29.14	-92.312	-95.299	16.696
UNCERTAINTY		0.03	0.03		0.130	0.130	0.023
400	7.375	195.41	188.03	28.91	-92.609	-96.276	12.572
500	11.706	201.89	190.18	29.22	-92.952	-97.154	10.150
600	14.663	207.26	192.60	29.68	-93.285	-97.963	8.528
700	16.844	211.87	195.03	30.19	-93.596	-98.716	7.366
800	18.544	215.93	197.39	30.69	-93.878	-99.427	6.492
900	19.922	219.58	199.66	31.19	-94.132	-100.108	5.810
1000	21.073	222.89	201.82	31.68	-94.362	-100.762	5.263
1100	22.060	225.93	203.87	32.16	-94.563	-101.384	4.814
1200	22.921	228.75	205.83	32.62	-94.744	-101.998	4.440
1300	23.684	231.38	207.70	33.07	-94.903	-102.599	4.122
1400	24.371	233.85	209.48	33.52	-95.041	-103.196	3.850
1500	24.995	236.17	211.18	33.95	-95.161	-103.763	3.613
1600	25.568	238.38	212.81	34.38	-95.263	-104.336	3.406
1700	26.099	240.47	214.37	34.80	-95.347	-104.893	3.223
1800	26.593	242.48	215.89	35.21	-95.416	-105.469	3.061

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	8.640 kJ	MOLAR VOLUME	2478.9200 J/bar 24789.200 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

HEAT CAPACITY EQUATION

$$C_p^0 = 32.325 + 3.3258 \times 10^{-3} T - 1.3590 \times 10^{-6} T^2 + 3.2835 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	247	215	215	COMPILED 6- 2-76
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SYLVITE FORMULA WEIGHT 74.551

KCl: Crystals 298.15 to melting point 1043 K. Liquid 1043 to fictive boiling point 1750 K.

TEMP. K					FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	82.59	82.59	51.29	-436.470	-408.554	71.577
UNCERTAINTY		0.20	0.20		0.140	0.140	0.025
400	13.375	98.01	84.63	53.41	-438.418	-398.638	52.057
500	21.506	110.06	88.55	54.64	-437.908	-388.743	40.612
600	27.145	120.15	93.00	56.11	-437.226	-378.979	32.993
700	31.411	128.93	97.52	57.99	-436.356	-369.331	27.560
800	34.872	136.82	101.95	60.27	-435.275	-359.828	23.494
900	37.833	144.07	106.24	62.87	-433.974	-350.480	20.341
1000	40.482	150.84	110.36	65.76	-432.428	-341.278	17.827
1043	41.640	153.95	112.31	67.07	-511.382	-336.959	16.875
1043	66.841	179.15	112.31	66.94	-485.098	-336.959	16.875
1100	67.191	182.80	115.61	66.94	-483.160	-329.331	15.639
1200	67.725	189.20	121.47	66.94	-479.761	-315.497	13.733
1300	68.177	195.10	126.92	66.94	-476.364	-301.955	12.133
1400	68.564	200.54	131.97	66.94	-472.973	-288.646	10.770
1500	68.899	205.60	136.70	66.94	-469.583	-275.576	9.596
1600	69.193	210.37	141.18	66.94	-466.198	-262.786	8.579
1700	69.452	214.80	145.35	66.94	-462.816	-250.124	7.685

MELTING POINT	1043	K	BOILING POINT	1750	K
ENTHALPY OF MELTING	26.284 kJ		ENTHALPY OF VAPORIZATION	155.394 kJ	
$H_{298}^0 - H_0^0$	11.368 kJ		MOLAR VOLUME	3.7524 J/bar 37.524 cm <sup>3</sup>	

## TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = -24.516 + 4.8522 \times 10^{-2} T + 1.3710 \times 10^{-3} T^{-0.5} - 1.6054 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1043 K)

REFERENCE	247	215	215	COMPILED
	173			5-28-76

CHLOROMAGNESITE FORMULA WEIGHT 95.211

HgCl<sub>2</sub>: Crystals 298.15 to melting point 987 K. Liquid 987 to boiling point 1710 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	89.62	89.62	71.04	-641.320	-591.785	103.679
UNCERTAINTY		0.84	0.84		0.460	0.544	0.095
400	18.750	111.22	92.47	75.64	-639.951	-575.067	75.096
500	30.394	128.39	98.00	78.17	-638.495	-559.015	58.400
600	38.508	142.80	104.29	79.93	-637.004	-543.254	47.295
700	44.529	155.23	110.70	81.33	-635.515	-527.749	39.381
800	49.205	166.17	116.97	82.53	-634.042	-512.458	33.460
900	52.967	175.96	122.99	83.63	-632.598	-497.354	28.866
987	55.798	184.01	128.21	84.52	-640.229	-483.881	25.608
987	99.461	227.67	128.21	92.47	-597.134	-483.881	25.608
1000	99.370	228.82	129.45	92.47	-596.844	-482.356	25.196
1100	98.743	237.65	138.91	92.47	-594.610	-471.025	22.367
1200	98.219	245.68	147.46	92.47	-592.389	-459.876	20.018
1300	97.777	253.09	155.31	92.47	-590.174	-448.928	18.038
1400	97.398	259.91	162.51	92.47	-714.928	-434.507	16.212
1500	97.069	266.31	169.24	92.47	-711.544	-414.633	14.439
1600	96.781	272.29	175.51	92.47	-708.167	-394.956	12.894
1700	96.527	277.90	181.37	92.47	-704.798	-375.491	11.537

MELTING POINT	987 K	BOILING POINT	1710 K
ENTHALPY OF MELTING	43.095 kJ	ENTHALPY OF VAPORIZATION	156.230 kJ
H <sub>298}^0 - H<sub>0}^0</sub></sub>	13.770 kJ	MOLAR VOLUME	4.0810 J/bar 40.810 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 76.903 + 8.4955 \times 10^{-3} T - 7.4631 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 987 K)

REFERENCE	169	120	214	COMPILED
		247	247	6-9-76

## SCACCHITE

FORMULA WEIGHT 125.844

MnCl<sub>2</sub>: Crystals 298.15 to melting point 923 K. Liquid 923 to 1400 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	118.24	118.24	73.01	-481.290	-440.488	77.172
UNCERTAINTY		0.21	0.21		0.837	0.879	0.154
400	19.175	140.35	121.17	77.25	-479.930	-426.762	55.730
500	31.068	157.88	126.81	79.80	-478.557	-413.622	43.211
600	39.357	172.61	133.25	81.73	-477.211	-400.765	34.890
700	45.529	185.33	139.80	83.37	-475.898	-388.124	28.962
800	50.352	196.56	146.21	84.85	-474.610	-375.674	24.529
900	54.267	206.64	152.37	86.24	-473.332	-363.388	21.091
923	55.167	209.60	154.44	88.56	-472.767	-361.187	20.440
923	95.828	250.26	154.44	94.56	-457.696	-361.187	20.440
1000	95.730	257.19	161.46	94.56	-436.085	-354.396	18.512
1100	95.624	266.19	170.56	94.56	-434.169	-346.296	16.444
1200	95.535	274.43	178.89	94.56	-432.306	-338.405	14.730
1300	95.459	282.00	186.54	94.56	-430.495	-330.657	13.286
1400	95.395	288.99	193.59	94.56	-431.014	-322.961	12.050

MELTING POINT	923 K	BOILING POINT	K
ENTHALPY OF MELTING	37.530 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	15.071 kJ	MOLAR VOLUME	4.2110 J/bar 42.110 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
H. P. DELTA 1517 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 76.261 + 1.1914 \times 10^{-2} T - 6.0475 \times 10^{-5} T^2$$

(EQUATION VALID FROM 298 - 923 K)

REFERENCE	169	34	214	COMPILED
			147	6- 9-76

SALAMMONIAC FORMULA WEIGHT 53.491

NH<sub>4</sub>Cl: Alpha crystals 298.15 to 457.7 K. Beta crystals 457.7 to melting point 793.2 K. Decomposition temperature (from differential thermal analysis) is 611.4 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	95.02	95.02	86.65	-315.190	-203.776	35.701
UNCERTAINTY		0.40	0.40		0.290	0.290	0.051
400	24.172	122.80	98.63	102.97	-314.694	-165.748	21.645
457.7	34.470	137.06	102.59	110.65	-313.810	-145.435	16.598
457.7	43.099	145.69	102.59	86.03	-309.860	-145.435	16.598
500	46.920	153.49	106.57	90.50	-310.002	-129.015	13.478
600	55.117	170.98	115.86	101.67	-309.556	-92.837	8.082
700	62.563	187.49	124.92	112.80	-308.062	-56.822	4.240

MELTING POINT	793.20 K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	22.698 kJ	MOLAR VOLUME	3.5060 J/bar 35.060 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

REFERENCE 247 215 215 COMPILED  
7-24-76

## HALITE

FORMULA WEIGHT 58.443

NaCl: Crystals 298.15 to melting point 1073.8 K. Liquid 1073.8 to fictive boiling point 1791 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	72.12	72.12	50.51	-411.260	-384.212	67.313
UNCERTAINTY		0.21	0.21		0.110	0.110	0.019
400	13.100	87.22	74.12	52.34	-413.461	-374.837	48.949
500	21.124	99.09	77.97	54.14	-413.024	-365.229	38.155
600	26.775	109.12	82.34	55.94	-412.352	-355.730	30.969
700	31.070	117.88	86.81	57.73	-411.456	-346.356	25.846
800	34.515	125.71	91.20	59.53	-410.352	-337.136	22.013
900	37.389	132.82	95.43	61.33	-409.064	-328.064	19.040
1000	39.877	139.37	99.49	63.12	-407.593	-319.133	16.670
1073.80	41.702	144.41	102.41	64.45	-380.693	-313.098	15.231
1073.80	67.925	170.33	102.41	68.55	-352.535	-313.098	15.231
1100	67.934	171.89	103.96	68.46	-377.527	-310.967	14.767
1200	67.964	177.83	109.87	68.14	-472.918	-302.951	13.187
1300	67.965	183.27	115.30	67.82	-470.082	-288.905	11.608
1400	67.943	188.29	120.35	67.50	-467.285	-275.089	10.264
1500	67.903	192.93	125.03	67.17	-464.521	-261.445	9.104
1600	67.847	197.26	129.41	66.85	-461.794	-248.002	8.096
1700	67.779	201.30	133.52	66.53	-459.103	-234.720	7.212

MELTING POINT	1073.8 K	BOILING POINT	1791 K
ENTHALPY OF MELTING	28.158 kJ	ENTHALPY OF VAPORIZATION	164.787 kJ
$H_{298}^0 - H_0^0$	10.611 kJ	MOLAR VOLUME	2.7015 J/bar 27.015 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 45.151 + 1.7974 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 1073.8 K)

$$C_P^0 = 72.008 - 3.2228 \times 10^{-3} T$$

(EQUATION VALID FROM 1073.8 - 1791 K)

REFERENCE	247	215	215	COMPILED 6- 2-76
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NICKEL CHLORIDE

FORMULA WEIGHT 129.606

NiCl<sub>2</sub>: Crystals 298.15 to melting point 1303 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	97.66	97.66	71.67	-305.330	-259.030	45.381
UNCERTAINTY		0.21	0.21		0.080	0.080	0.014
400	19.150	119.71	100.56	77.20	-303.987	-243.411	31.786
500	30.888	137.09	106.20	78.33	-302.727	-228.422	23.863
600	38.840	151.41	112.57	78.88	-301.768	-213.652	18.600
700	44.616	163.63	119.01	79.73	-300.831	-199.030	14.852
800	49.082	174.36	125.28	81.05	-299.586	-184.578	12.052
900	52.733	184.01	131.28	82.86	-298.256	-170.285	9.883
1000	55.853	192.85	137.00	85.10	-296.846	-156.136	8.156
1100	58.628	201.08	142.45	87.72	-295.313	-142.138	6.750
1200	61.172	208.84	147.67	90.65	-293.610	-128.286	5.584
1300	63.562	216.22	152.66	93.87	-291.684	-114.584	4.604

MELTING POINT	1303 K	BOILING POINT	K
ENTHALPY OF MELTING	77.280 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	14.385 kJ	MOLAR VOLUME	3.6700 J/bar 36.700 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

NICKEL..... CURIE P. 631, M. P. 1726 K.

HEAT CAPACITY EQUATION

$$C_P^0 = - 50.781 + 5.7481 \times 10^{-2} T + 2.6078 \times 10^{-3} T^{0.5} - 4.0637 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1303 K)

REFERENCE	40	263	263	COMPILED
				6- 2-76

## COTUNNITE

FORMULA WEIGHT 278.106

PbCl<sub>2</sub>: Crystals 298.15 to melting point 768 K. Liquid 768 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	135.98	135.98	73.15	-359.400	-314.033	55.017
UNCERTAINTY		2.09	2.09		0.293	0.711	0.125
400	19.550	158.50	138.95	79.95	-357.861	-298.761	39.014
500	32.110	176.85	144.74	84.48	-355.979	-284.194	29.690
600	41.130	192.56	151.43	87.82	-353.871	-270.027	23.508
700	47.993	206.30	158.31	90.42	-356.470	-255.432	19.061
768	51.698	215.07	163.38	91.89	-354.936	-245.970	16.729
768	82.752	246.13	163.38	113.80	-331.087	-245.970	16.729
800	83.994	250.41	166.42	113.80	-329.592	-242.234	15.816
900	87.306	263.80	176.50	113.80	-324.920	-231.581	13.441
1000	89.956	275.77	185.81	113.80	-320.229	-221.436	11.567

MELTING POINT	768 K	BOILING POINT	K
ENTHALPY OF MELTING	23.849 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	16.941 kJ	MOLAR VOLUME	4.7090 J/bar 47.090 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

LEAD..... H. P. 600.6, B. P. 2021 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.2287 \times 10^2 - 8.5847 \times 10^2 T^{-0.5}$$

(EQUATION VALID FROM 298 - 768 K)

REFERENCE	115	120	247	COMPILED
		215	215	6- 9-76

TITANIUM TRICHLORIDE FORMULA WEIGHT 154.259

TiCl<sub>3</sub>: Crystals 298.15 to 1200 K. The free energy for the reaction TiCl<sub>3</sub> (c) = TiCl<sub>3</sub> (g) approaches zero at 1104.1 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	139.75	139.75	97.16	-721.740	-654.507	114.667
UNCERTAINTY		1.26	1.26		4.180	5.020	0.879
400	25.025	168.61	143.58	99.26	-719.646	-631.862	82.513
500	40.030	190.93	150.90	100.87	-717.680	-610.145	63.742
600	50.285	209.45	159.16	102.22	-715.757	-588.822	51.262
700	57.790	225.29	167.50	103.41	-713.870	-567.808	42.371
800	63.560	239.17	175.61	104.49	-712.009	-547.074	35.720
900	68.167	251.54	183.37	105.49	-710.173	-526.573	30.562
1000	71.942	262.70	190.76	106.43	-708.371	-506.271	26.445
1100	75.118	272.89	197.77	107.33	-706.592	-486.142	23.085
1200	77.838	282.26	204.42	108.19	-708.896	-466.021	20.285

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.7300 J/bar 57.300 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.0609 \times 10^2 + 6.2428 \times 10^{-3} T - 1.8660 \times 10^2 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE 141 247 247 COMPILED  
6- 2-76

## URANIUM TRICHLORIDE

FORMULA WEIGHT 344.388

UCl<sub>3</sub>: Crystals 298.15 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	158.95	158.95	101.73	-891.190	-823.820	144.330
UNCERTAINTY		0.40	0.40		4.000	5.000	0.876
400	26.125	188.69	162.57	104.23	-888.957	-800.997	104.600
500	41.912	212.14	170.23	105.71	-886.882	-779.257	81.409
600	52.643	231.52	178.88	107.02	-885.031	-757.910	65.982
700	60.569	248.18	187.61	109.43	-883.364	-736.854	54.985
800	66.891	263.01	196.12	113.09	-881.785	-716.025	46.752
900	72.278	276.60	204.32	117.92	-880.223	-695.417	40.361
1000	77.130	289.32	212.19	123.75	-881.003	-674.803	35.248

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	6.2040 J/bar 62.040 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

URANIUM.... ALPHA-BETA 941, BETA-GAMMA 1048, M. P. 1405 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = -1.7529 \times 10^2 + 0.13399 T + 5.4565 \times 10^3 T^{-0.5} - 7.5036 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	70	70	89 233	COMPILED 7- 1-76
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URANIUM TETRACHLORIDE

FORMULA WEIGHT 379.841

UCl<sub>4</sub>: Crystals 298.15 to 700 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	196.60	196.60	119.89	-1018.390	-928.850	162.731
UNCERTAINTY		0.50	0.50		3.000	3.000	0.526
400	31.625	233.05	201.42	127.29	-1015.723	-898.855	117.379
500	51.174	261.90	210.73	131.32	-1013.001	-869.951	90.884
600	64.878	286.21	221.33	135.62	-1010.255	-841.596	73.268
700	75.347	307.50	232.15	140.87	-1007.420	-813.708	60.720

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	7.7600 J/bar 77.600 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

URANIUM.... ALPHA-BETA 941, BETA-GAMMA 1048, H. P. 1405 K.

HEAT CAPACITY EQUATION

$$C_p^0 = - 80.231 + 0.12983 T + 3.6987 \times 10^{-3} T^{-0.5} - 4.6948 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 700 K)

REFERENCE	70	70	89	COMPILED
			233	8-17-76

VANADIUM DICHLORIDE FORMULA WEIGHT 121.847

VCl<sub>2</sub>: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	97.07	97.07	72.20	-451.870	-405.681	71.074
UNCERTAINTY		1.26	1.26		8.500	8.500	1.489
400	18.775	118.73	99.95	75.06	-450.498	-390.118	50.944
500	30.228	135.68	105.45	76.84	-449.107	-375.177	39.195
600	38.118	149.82	111.70	78.27	-447.691	-360.523	31.386
700	43.949	161.98	118.03	79.57	-446.246	-346.104	25.827
800	48.479	172.69	124.21	80.81	-444.773	-331.901	21.671
900	52.144	182.28	130.14	82.03	-443.272	-317.884	18.450
1000	55.189	190.98	135.79	83.24	-441.761	-304.031	15.881
1100	57.794	198.97	141.18	84.45	-440.231	-290.323	13.786
1200	60.065	206.37	146.30	85.66	-438.695	-276.766	12.047
1300	62.081	213.28	151.20	86.87	-437.158	-263.335	10.581

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	J/bar

TRANSITIONS IN REFERENCE STATE ELEMENTS

VANADIUM... M. P. 2175 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 66.755 + 1.3045 \times 10^{-2} T + 1.2465 \times 10^{-5} T^2 - 5.0348 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	125	120	264	COMPILED 5-28-76
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VANADIUM TRICHLORIDE

FORMULA WEIGHT 157.300

VCl<sub>3</sub>: Crystals 298.15 to 900 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	130.96	130.96	93.16	-580.740	-511.399	89.595
UNCERTAINTY		1.70	1.70		0.850	0.850	0.149
400	24.525	159.21	134.68	98.88	-578.834	-487.994	63.726
500	39.752	181.67	141.92	102.26	-576.764	-465.524	48.633
600	50.362	200.52	150.16	104.41	-574.579	-443.480	38.609
700	58.189	216.72	158.53	105.79	-572.349	-421.800	31.475
800	64.196	230.91	166.71	106.64	-570.120	-400.449	26.147
900	68.944	243.50	174.56	107.11	-567.935	-379.376	22.018

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	5.4480 J/bar 54.480 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

VANADIUM... M. P. 2175 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 148.86 - 1.3301 \times 10^{-2} T - 8.9326 \times 10^{-5} T^{-0.5}$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	125	120	264	COMPILED 6-29-76
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## ALUMINUM TRIFLUORIDE

FORMULA WEIGHT 83.977

$\text{AlF}_3$ : Alpha crystals 298.15 to 728 K. Beta crystals 728 to 1800 K. The dissociation temperature is 1549 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	66.48	66.48	75.13	-1510.400	-1431.076	250.720
UNCERTAINTY		0.42	0.42		1.300	1.300	0.228
400	20.750	90.34	69.59	86.07	-1509.575	-1404.081	183.355
500	34.422	110.21	75.79	92.00	-1508.342	-1377.849	143.944
600	44.495	127.49	82.99	97.82	-1506.806	-1351.895	117.693
700	52.577	143.06	90.48	104.48	-1504.895	-1326.220	98.964
728	54.442	147.97	93.52	106.52	-1504.252	-1319.660	94.687
728	55.265	148.79	93.52	98.16	-1503.653	-1319.660	94.687
800	59.237	157.22	97.98	98.88	-1502.743	-1300.856	84.938
900	63.700	168.93	105.23	99.87	-1501.479	-1275.706	74.040
1000	67.364	179.50	112.14	100.87	-1511.024	-1249.924	65.290
1100	70.455	189.16	118.71	101.86	-1509.672	-1223.864	58.117
1200	73.113	198.07	124.96	102.85	-1508.259	-1197.965	52.146
1300	75.439	206.34	130.90	103.85	-1506.783	-1172.136	47.097
1400	77.507	214.07	136.56	104.84	-1505.233	-1146.454	42.775
1500	79.359	221.34	141.98	105.83	-1503.621	-1120.895	39.033
1600	81.045	228.20	147.15	106.83	-1501.935	-1095.438	35.763
1700	82.591	234.70	152.11	107.82	-1500.174	-1070.092	32.880
1800	84.020	240.90	156.88	108.81	-1498.339	-1044.848	30.321

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	2.6150 J/bar 26.150 $\text{cm}^3$

## TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = -1.4615 \times 10^{-2} + 0.15039 T + 4.1536 \times 10^{-3} T^{-0.5} - 5.6988 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 728 K)

$$C_P^0 = 90.932 + 9.9337 \times 10^{-3} T$$

(EQUATION VALID FROM 728 - 1800 K)

REFERENCE	51	247	247	COMPILED
	181	215	215	8-11-76



FLUORITE FORMULA WEIGHT 78.077

CaF<sub>2</sub>: Crystals I 298.15 to transition point 1424 K. Crystals II 1424 to melting point 1691 K. Liquid 1691 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	68.87	68.87	68.59	-1229.260	-1176.920	206.192
UNCERTAINTY		0.34	0.34		0.420	0.420	0.074
400	18.300	89.94	71.64	74.09	-1227.845	-1159.245	151.383
500	29.710	106.75	77.04	76.50	-1226.375	-1142.270	119.333
600	37.678	120.88	83.20	78.54	-1224.961	-1125.583	97.991
700	43.673	133.15	89.48	80.80	-1223.625	-1109.126	82.764
800	48.474	144.11	95.64	83.42	-1223.080	-1092.768	71.351
900	52.522	154.10	101.58	86.39	-1221.729	-1076.550	62.482
1000	56.068	163.37	107.30	89.68	-1220.523	-1060.493	55.395
1100	59.283	172.09	112.81	93.24	-1219.416	-1044.549	49.602
1200	62.268	180.36	118.09	97.02	-1225.326	-1028.083	44.751
1300	65.094	188.28	123.19	101.01	-1222.144	-1011.765	40.653
1400	67.807	195.92	128.11	105.17	-1218.574	-995.722	37.151
1424	68.402	198.05	129.65	105.19	-1217.706	-992.219	36.396
1424	71.722	201.37	129.65	122.88	-1212.978	-992.219	36.396
1500	74.363	207.44	133.08	123.68	-1208.715	-980.240	34.135
1600	77.456	215.43	137.98	124.73	-1203.106	-965.194	31.510
1691	80.057	222.42	142.36	125.68	-1184.042	-952.223	29.414
1691	97.624	239.99	142.36	100.00	-1154.336	-952.223	29.414
1700	97.635	240.50	142.86	100.00	-1167.850	-950.673	29.211
1800	97.743	246.19	148.45	100.00	-1318.202	-934.620	27.122

MELTING POINT	1691 K	BOILING POINT	K
ENTHALPY OF MELTING	29.706 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	2.4542 J/bar 24.542 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

HEAT CAPACITY EQUATION

$$C_P^0 = - 24.692 + 5.8095 \times 10^{-2} T + 1.8706 \times 10^{-5} T^{0.5} - 2.8774 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1424 K)

REFERENCE 175 215 215 COMPILED 6-15-76

## SELLAITE

FORMULA WEIGHT 62.302

HgF<sub>2</sub>: Crystals 298.15 to melting point 1536 K. Liquid 1536 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	57.25	57.25	61.59	-1124.200	-1071.064	187.647
UNCERTAINTY		0.42	0.42		1.200	1.200	0.210
400	16.700	76.48	59.78	68.75	-1123.403	-1053.027	137.512
500	27.520	92.26	64.74	72.46	-1122.369	-1035.549	108.184
600	35.225	105.70	70.48	74.90	-1121.261	-1018.289	88.650
700	41.029	117.39	76.36	76.73	-1120.140	-1001.217	74.712
800	45.587	127.73	82.14	78.24	-1119.031	-984.296	64.268
900	49.289	137.03	87.74	79.56	-1117.949	-967.523	56.154
1000	52.378	145.47	93.09	80.76	-1125.846	-950.106	49.629
1100	55.010	153.22	98.21	81.89	-1124.715	-932.578	44.285
1200	57.295	160.39	103.10	82.97	-1123.501	-915.170	39.836
1300	59.310	167.08	107.77	84.01	-1122.204	-897.863	36.077
1400	61.107	173.34	112.23	85.02	-1247.790	-877.055	32.723
1500	62.737	179.24	116.50	86.01	-1245.141	-850.670	29.623
1536	63.233	181.66	118.42	87.02	-1244.243	-841.187	28.606
1536	101.096	219.52	118.42	94.56	-1186.085	-841.187	28.606
1600	100.834	223.19	122.35	94.56	-1183.837	-827.257	27.007
1700	100.465	228.92	128.45	94.56	-1180.324	-805.082	24.737
1800	100.137	234.36	134.22	94.56	-1176.827	-783.182	22.727

MELTING POINT	1536 K	BOILING POINT	2630 K
ENTHALPY OF MELTING	58.158 kJ	ENTHALPY OF VAPORIZATION	240.162 kJ
$H_{298}^0 - H_0^0$	9.983 kJ	MOLAR VOLUME	1.9610 J/bar 19.610 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 72.887 + 9.1200 \times 10^{-3} T - 1.2460 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1536 K)

REFERENCE	175	247	215	COMPILED 6- 9-76
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VILLIAUMITE

FORMULA WEIGHT 41.988

NaF: Crystals 298.15 to melting point 1269 K. Liquid 1269 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	51.30	51.30	46.85	-576.550	-546.319	95.713
UNCERTAINTY		0.08	0.08		0.670	0.670	0.117
400	12.350	65.54	53.19	49.72	-578.927	-535.833	69.973
500	19.980	76.80	56.82	51.18	-578.665	-525.087	54.856
600	25.292	86.25	60.96	52.53	-578.236	-514.411	44.784
700	29.287	94.45	65.16	54.02	-577.641	-503.805	37.595
800	32.481	101.77	69.29	55.71	-576.877	-493.309	32.210
900	35.167	108.44	73.27	57.58	-575.934	-482.919	28.028
1000	37.507	114.61	77.10	59.63	-574.818	-472.648	24.689
1100	39.616	120.40	80.78	61.81	-573.526	-462.487	21.962
1200	41.562	125.87	84.31	64.12	-669.452	-450.400	19.605
1269	43.067	129.83	86.76	65.77	-667.412	-437.699	18.017
1269	69.179	155.94	86.76	68.51	-634.275	-437.699	18.017
1300	69.165	157.51	88.35	68.51	-633.385	-433.078	17.401
1400	69.121	162.58	93.46	68.51	-630.513	-417.764	15.587
1500	69.077	167.31	98.23	68.51	-627.660	-402.676	14.022
1600	69.042	171.73	102.69	68.51	-624.810	-387.770	12.659
1700	69.011	175.88	106.87	68.51	-621.970	-373.039	11.462
1800	68.983	179.80	110.82	68.51	-619.139	-358.488	10.403

MELTING POINT	1269	K	BOILING POINT	K
ENTHALPY OF MELTING	33.137	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	8.485	kJ	MOLAR VOLUME	1.4984 J/bar 14.984 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = -2.6123 + 3.3468 \times 10^{-2} T + 9.5415 \times 10^{-2} T^{-0.5} - 1.4023 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1269 K)

REFERENCE	181	215	215	COMPILED 6- 9-76
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## CRYOLITE

FORMULA WEIGHT 209.942

$\text{Na}_3\text{AlF}_6$ : Crystals 298.15 to 1500 K. Cryolite dissociates above 1279 K  
presumably by the reaction  $\text{Na}_3\text{AlF}_6 = \text{NaAlF}_4 + 2\text{NaF}$ .

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K			
298.15	0.000	238.45	238.45	215.72	-3309.544	-3144.915	550.978
UNCERTAINTY		1.67	1.67		4.180	4.300	0.753
400	57.350	304.50	247.15	233.86	-3316.030	-3088.271	403.289
500	94.176	358.33	264.15	248.90	-3313.924	-3031.559	316.706
600	121.155	404.97	283.82	263.11	-3310.537	-2975.388	259.032
700	142.429	446.58	304.15	276.99	-3305.921	-2919.857	217.883
800	160.109	484.46	324.35	290.72	-3300.126	-2865.079	187.071
838	165.721	499.38	333.66	295.92	-3291.226	-2845.884	177.392
838	176.292	509.95	333.66	262.96	-3282.367	-2845.884	177.392
900	183.456	528.25	344.79	272.55	-3285.947	-2811.727	163.189
1000	193.138	557.77	364.63	288.02	-3291.721	-2758.551	144.093
1100	202.467	585.94	383.47	303.49	-3285.264	-2705.476	128.473
1200	211.531	613.01	401.48	318.96	-3569.632	-2646.975	115.220
1285	217.696	635.45	417.75	332.11	-3561.380	-2583.536	105.020
1285	304.665	722.42	417.75	396.91	-3449.625	-2583.536	105.020
1300	305.729	726.83	421.10	396.91	-3446.797	-2573.577	103.408
1400	312.243	756.24	444.00	396.91	-3427.946	-2507.123	93.542
1500	317.887	783.63	465.74	396.91	-3409.151	-2442.014	85.039
1600	322.826	809.24	486.41	396.91	-3390.413	-2378.156	77.639
1700	327.184	833.31	506.13	396.91	-3371.726	-2315.501	71.147
1800	331.058	855.99	524.93	396.91	-3353.093	-2253.891	65.407

MELTING POINT	1285	K	BOILING POINT	K
ENTHALPY OF MELTING	111.755	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	38.100	kJ	MOLAR VOLUME	7.0810 J/bar 70.810 $\text{cm}^3$

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

ALUMINUM... M. P. 933 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.8277 \times 10^2 + 13.542 T - 1.9693 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 838 K)

$$C_P^0 = 1.3331 \times 10^2 + 0.15471 T$$

(EQUATION VALID FROM 838 - 1285 K)

REFERENCE	181	247	247	COMPILED 8-11-76
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URANIUM TETRAFLUORIDE

FORMULA WEIGHT 314.023

UF<sub>4</sub>: Crystals 298.15 to melting point 1330 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	151.67	151.67	116.02	-1853.500	-1762.800	308.837
UNCERTAINTY		0.17	0.17		5.000	5.100	0.894
400	30.300	186.60	156.30	120.86	-1850.867	-1732.227	226.207
500	48.598	213.77	165.17	122.64	-1848.513	-1702.848	177.896
600	61.072	236.27	175.20	124.29	-1846.463	-1673.915	145.728
700	70.249	255.59	185.34	126.42	-1844.689	-1645.301	122.774
800	77.432	272.64	195.21	129.11	-1843.144	-1616.912	105.574
900	83.344	288.02	204.68	132.30	-1841.808	-1588.720	92.207
1000	88.422	302.15	213.73	135.95	-1843.064	-1560.514	81.513
1100	92.923	315.29	222.37	139.97	-1845.558	-1532.102	72.754
1200	97.022	327.66	230.64	144.31	-1842.705	-1503.754	65.457
1300	100.835	339.39	238.55	148.92	-1839.451	-1475.606	59.291

MELTING POINT	1330 K	BOILING POINT	K
ENTHALPY OF MELTING	42.803 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	22.552 kJ	MOLAR VOLUME	4.6880 J/bar 46.880 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

URANIUM.... ALPHA-BETA 941, BETA-GAMMA 1048, M. P. 1405 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -8.5443 + 7.0363 \times 10^{-2} T + 2.4522 \times 10^{-5} T^{-0.5} - 3.4164 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	70	70	233	COMPILED 6- 8-76
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## IODARGYRITE

FORMULA WEIGHT 234.772

AgI: Hexagonal crystals 298.15 to 423 K. Cubic crystals 423 to 831 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K			
298.15	0.000	115.48	115.48	56.82	-61.840	-66.254	11.607
UNCERTAINTY		1.67	1.67		1.674	1.757	0.308
400	15.167	132.93	117.76	28.38	-69.313	-67.538	8.820
423	17.903	136.56	118.68	28.62	-69.350	-67.447	8.329
423	32.449	151.13	118.68	56.48	-63.188	-67.447	8.329
500	36.150	160.54	124.39	56.48	-83.929	-66.270	6.924
600	39.538	170.88	131.38	56.48	-82.827	-62.869	5.473
700	41.960	179.54	137.58	56.48	-81.770	-59.593	4.447
800	43.775	187.07	143.29	56.48	-80.798	-56.484	3.688

MELTING POINT	831	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	4.1301 J/bar 41.301 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SILVER..... M. P. 1234 K.

IODINE..... M. P. 386.75, B. P. 458 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 24.351 + 1.0083 \times 10^{-2} T$$

(EQUATION VALID FROM 298 - 423 K)

REFERENCE	115	120	263	263	COMPILED
		263			7-24-76

COCCINITE

FORMULA WEIGHT 454.399

HgI<sub>2</sub>: Crystals I 298.15 to 403 K. Crystals II 403 to melting point 523 K.  
Liquid 523 to 627 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	181.33	181.33		-105.437	-102.203	17.906
UNCERTAINTY		6.28	6.28		1.674	2.552	0.447
400	20.334	204.77	184.44	82.01	-121.977	-100.475	13.121
500	38.108	229.77	191.66	84.12	-161.813	-91.682	9.578
600	79.775	282.42	202.64	102.09	-139.467	-79.817	6.949

MELTING POINT	523	K	BOILING POINT	627	K
ENTHALPY OF MELTING	18.828	kJ	ENTHALPY OF VAPORIZATION	59.166	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	7.1840	J/bar 71.840 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MERCURY.... B. P. 629 K.

IODINE..... M. P. 386.75, B. P. 458 K.

REFERENCE	115	263	263	COMPILED
	32	32	247	7-24-76

## WITHERITE

FORMULA WEIGHT 197.349

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 BaCO<sub>3</sub>: Orthorhombic crystals 298.15 to 1079 K. Tetragonal crystals 1079 to  
 1241 K. Cubic crystals 1241 to 1600 K.  
 =====

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	GIBBS FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>p</sub> <sup>0</sup> J/mol·K			
298.15	0.000	112.13	112.13	85.35	-1210.850	-1132.210	198.359
UNCERTAINTY		2.09	2.09		2.230	2.240	0.392
400	23.575	139.25	115.68	98.42	-1210.071	-1105.461	144.359
500	39.400	162.13	122.73	106.59	-1209.550	-1079.381	112.763
600	51.173	182.17	131.00	113.36	-1209.498	-1053.335	91.701
700	60.506	200.12	139.61	119.57	-1208.319	-1027.417	76.667
800	68.264	216.48	148.22	125.54	-1207.305	-1001.631	65.400
900	74.956	231.60	156.64	131.38	-1205.493	-976.011	56.646
1000	80.885	245.74	164.85	137.15	-1203.282	-950.629	49.656
1079	85.640	256.91	171.27	141.68	-1209.054	-930.172	45.030
1079	101.917	273.19	171.27	154.81	-1191.491	-930.172	45.030
1100	102.926	276.02	173.09	154.81	-1190.676	-924.964	43.923
1200	107.250	289.49	182.24	154.81	-1186.910	-900.986	39.219
1241	108.734	295.01	186.28	154.81	-1185.454	-891.519	37.525
1241	111.254	297.54	186.28	158.98	-1182.328	-891.519	37.525
1300	113.422	304.49	191.07	158.98	-1179.876	-877.427	35.256
1400	116.679	316.28	199.60	158.98	-1175.722	-854.351	31.876
1500	119.495	327.24	207.74	158.98	-1171.549	-831.516	28.956
1600	121.963	337.50	215.54	158.98	-1167.421	-808.986	26.411

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	4.5810 J/bar 45.810 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

BARUM..... ALPHA-BETA 582, BETA-GAMMA 768, M. P. GAMMA 1002,  
 B. P. 2169 K.

## HEAT CAPACITY EQUATIONS

$$C_p^0 = 81.001 + 5.6484 \times 10^{-2} T - 3.3107 \times 10^{-5} T^2$$

(EQUATION VALID FROM 298 - 1079 K)

REFERENCE	155	120	COMPILED 6-28-76
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WITHERITE

FORMULA WEIGHT 197.349

BaCO<sub>3</sub>: Orthorhombic crystals 298.15 to 1079 K. Tetragonal crystals 1079 to 1241 K. Cubic crystals 1241 to 1600 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	112.13	112.13	85.35	-269.240 *	-217.446 *	38.096
UNCERTAINTY		2.09	2.09		0.770	0.780	
400	23.575	139.25	115.68	98.42	-268.760 *	-199.799 *	26.091
500	39.400	162.13	122.73	106.59	-267.891 *	-182.656 *	19.082
600	51.173	182.17	131.00	113.36	-266.745 *	-165.711 *	14.426
700	60.506	200.12	139.61	119.57	-265.328 *	-148.987 *	11.117
800	68.264	216.48	148.22	125.54	-263.618 *	-132.473 *	8.649
900	74.956	231.60	156.64	131.38	-261.580 *	-116.201 *	6.744
1000	80.885	245.74	164.85	137.15	-259.193 *	-100.172 *	5.232
1079	85.640	256.91	171.27	141.68	-256.515 *	-87.766 *	4.249
1079	101.917	273.19	171.27	154.81	-238.953 *	-87.766 *	4.249
1100	102.926	276.02	173.09	154.81	-238.100 *	-84.701 *	4.022
1200	107.250	289.49	182.24	154.81	-234.038 *	-70.933 *	3.087
1241	108.734	295.01	186.28	154.81	-232.460 *	-65.740 *	2.767
1241	111.254	297.53	186.28	158.98	-229.333 *	-65.740 *	2.767
1300	113.422	304.49	191.07	158.98	-226.872 *	-57.623 *	2.315
1400	116.679	316.28	199.60	158.98	-222.700 *	-44.772 *	1.670
1500	119.495	327.24	207.74	158.98	-218.668 *	-32.188 *	1.121
1600	121.963	337.50	215.54	158.98	-214.757 *	-19.893 *	0.649

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	4.5810 J/bar 45.810 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

HEAT CAPACITY EQUATIONS

$$C_P^0 = 81.001 + 5.6484 \times 10^{-2} T - 3.3107 \times 10^{-5} T^2$$

(EQUATION VALID FROM 298 - 1079 K)

REFERENCE	155	120	4	COMPILED 6-28-76
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## ARAGONITE

FORMULA WEIGHT 100.089

CaCO<sub>3</sub>: Crystals 298.15 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	87.99	87.99	82.32	-1207.430	-1127.793	197.585
UNCERTAINTY		0.20	0.20		1.423	1.464	0.256
400	22.375	113.75	91.37	92.67	-1206.681	-1100.691	143.736
500	37.184	135.23	98.05	99.81	-1205.665	-1074.310	112.233
600	48.128	153.96	105.83	105.77	-1204.567	-1048.132	91.248
700	56.754	170.68	113.93	111.18	-1203.438	-1022.160	76.275
800	63.879	185.86	121.98	116.29	-1203.022	-996.251	65.049
900	69.978	199.84	129.86	121.23	-1201.749	-970.468	56.325
1000	75.346	212.87	137.52	126.07	-1200.573	-944.833	49.353

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.4150 J/bar 34.150 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, H. P. BETA 1112, B. P. 1755 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 81.533 + 4.5673 \times 10^{-2} T - 1.1405 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	115	243	214	COMPILED
				8- 2-76

ARAGONITE

FORMULA WEIGHT 100.089

CaCO<sub>3</sub>: Crystals 298.15 to 1000 K.

TEMP.	FORMATION FROM THE OXIDES						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	87.99	87.99	82.32	-178.831 *	-129.936 *	22.763
UNCERTAINTY		0.20	0.20		1.110	1.150	
400	22.375	113.75	91.37	92.67	-178.421 *	-113.284 *	14.793
500	37.184	135.23	98.05	99.81	-177.875 *	-97.060 *	10.140
600	48.128	153.96	105.83	105.77	-177.175 *	-80.959 *	7.048
700	56.754	170.68	113.93	111.18	-176.283 *	-64.996 *	4.850
800	63.879	185.86	121.98	116.29	-175.166 *	-49.165 *	3.210
900	69.978	199.84	129.86	121.23	-173.791 *	-33.497 *	1.944
1000	75.346	212.87	137.52	126.07	-172.136 *	-17.995 *	0.940

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.4150 J/bar 34.150 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

HEAT CAPACITY EQUATION

$$C_P^0 = 81.533 + 4.5673 \times 10^{-2} T - 1.1405 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	115	243	214	COMPILED
				8- 2-76

## CALCITE

FORMULA WEIGHT 100.089

CaCO<sub>3</sub>: Crystals 298.15 to 1400 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	91.71	91.71	83.47	-1207.370	-1128.842	197.769
UNCERTAINTY		0.20	0.20		1.339	1.381	0.242
400	23.175	118.36	95.18	97.00	-1206.301	-1102.155	143.927
500	38.750	140.88	102.13	104.54	-1204.822	-1076.292	112.440
600	50.180	160.43	110.25	109.87	-1203.276	-1050.723	91.474
700	59.021	177.70	118.68	114.16	-1201.791	-1025.427	76.519
800	66.150	193.19	127.04	117.88	-1201.145	-1000.238	65.309
900	72.089	207.27	135.18	121.28	-1199.789	-975.195	56.599
1000	77.170	220.22	143.05	124.48	-1198.689	-950.299	49.639
1100	81.610	232.23	150.62	127.54	-1197.837	-925.510	43.949
1200	85.563	243.45	157.89	130.52	-1204.162	-900.161	39.183

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.6934 J/bar 36.934 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 99.715 + 2.6920 \times 10^{-2} T - 2.1576 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	115	243	214	COMPILED 7-27-76
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CALCITE

FORMULA WEIGHT 100.089

CaCO<sub>3</sub>: Crystals 298.15 to 1400 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	91.71	91.71	83.47	-178.771 *	-130.985 *	22.947
UNCERTAINTY		0.20	0.20		1.000	1.040	
400	23.175	118.36	95.18	97.00	-178.041 *	-114.781 *	14.984
500	38.750	140.88	102.13	104.54	-177.032 *	-99.042 *	10.347
600	50.180	160.43	110.25	109.87	-175.884 *	-83.550 *	7.273
700	59.021	177.70	118.68	114.16	-174.636 *	-68.263 *	5.094
800	66.150	193.19	127.04	117.88	-173.289 *	-53.152 *	3.470
900	72.089	207.27	135.18	121.28	-171.831 *	-38.224 *	2.218
1000	77.170	220.22	143.05	124.48	-170.252 *	-23.461 *	1.225
1100	81.610	232.23	150.62	127.54	-168.538 *	-8.873 *	0.421
1200	85.563	243.45	157.89	130.52	-166.677 *	5.572 *	-0.243

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.6934 J/bar 36.934 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

HEAT CAPACITY EQUATION

$$C_P^0 = 99.715 + 2.6920 \times 10^{-2} T - 2.1576 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	115	243	214	COMPILED 7-27-76
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## DOLOMITE

FORMULA WEIGHT 184.403

CaMg(CO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	155.18	155.18	157.53	-2324.480	-2161.672	378.718
UNCERTAINTY		0.29	0.29		1.460	1.670	0.293
400	43.600	205.32	161.72	183.53	-2323.420	-2106.176	275.040
500	73.520	248.35	174.83	201.88	-2321.333	-2052.098	214.382
600	96.110	286.43	190.32	215.65	-2318.730	-1998.480	173.984
700	114.003	320.53	206.53	226.64	-2315.875	-1945.344	145.164
800	128.685	351.42	222.74	236.07	-2313.625	-1892.522	123.570
900	141.103	379.73	238.63	244.72	-2310.455	-1840.054	106.794
1000	151.888	405.96	254.07	253.14	-2316.263	-1787.193	93.354
1100	161.481	430.48	269.00	261.33	-2312.986	-1734.441	82.362

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	25.983 kJ	MOLAR VOLUME	6.4340 J/bar 64.340 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

MAGNESIUM.. M. P. 922, B. P. 1361 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 5.4788 \times 10^2 - 0.16759 T + 7.7076 \times 10^{-5} T^2 - 6.5479 \times 10^{-8} T^{-0.5} \\ + 2.8400 \times 10^{-6} T^{-2} \\ \text{(EQUATION VALID FROM 298 - 1100 K)}$$

REFERENCE	151	244	225	COMPILED 8- 2-76
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DOLOMITE

FORMULA WEIGHT 184.403

CaMg(CO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to 1000 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	155.18	155.18	157.53	-300.881 *	-200.249 *	35.081
UNCERTAINTY		0.29	0.29		1.120	1.130	
400	43.600	205.32	161.72	183.53	-300.071 *	-165.963 *	21.673
500	73.520	248.35	174.83	201.88	-298.556 *	-132.591 *	13.852
600	96.110	286.43	190.32	215.65	-296.484 *	-99.594 *	8.670
700	114.003	320.53	206.53	226.64	-293.963 *	-66.973 *	4.998
800	128.685	351.42	222.74	236.07	-291.056 *	-34.735 *	2.268
900	141.103	379.73	238.63	244.72	-287.758 *	-2.900 *	0.168
1000	151.888	405.96	254.07	253.14	-284.034 *	28.566 *	-1.492
1100	161.481	430.48	269.00	261.33	-279.822 *	59.614 *	-2.831

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	25.983 kJ	MOLAR VOLUME	6.4340 J/bar 64.340 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

HEAT CAPACITY EQUATION

$$C_P^0 = 5.4788 \times 10^2 - 0.16759 T + 7.7076 \times 10^{-5} T^2 - 6.5479 \times 10^3 T^{-0.5} + 2.8400 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1100 K)

REFERENCE	151	244	225	COMPILED 8- 2-76
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MAGNESITE

FORMULA WEIGHT 84.314

MgCO<sub>3</sub>: Crystals 298.15 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	65.09	65.09	76.09	-1113.280	-1029.480	180.361
UNCERTAINTY		0.14	0.14		1.339	1.381	0.242
400	21.400	89.67	68.27	90.57	-1112.899	-1000.885	130.703
500	36.206	110.94	74.73	99.92	-1111.963	-972.993	101.648
600	47.463	129.83	82.37	107.38	-1110.704	-945.305	82.296
700	56.500	146.89	90.39	113.96	-1109.190	-917.866	68.492
800	64.067	162.51	98.44	120.06	-1107.423	-890.652	58.154
900	70.611	176.99	106.38	125.89	-1105.399	-863.668	50.126
1000	76.426	190.54	114.11	131.54	-1112.036	-836.156	43.676

MELTING POINT

K

BOILING POINT

K

ENTHALPY OF MELTING

kJ

ENTHALPY OF VAPORIZATION

kJ

 $H_{298}^0 - H_0^0$ 

11.631 kJ

MOLAR VOLUME

2.8018 J/bar  
28.018 cm<sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 81.119 + 5.2254 \times 10^{-2} T - 1.8320 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE 115

95

220

COMPILED  
7-29-76



MAGNESITE

FORMULA WEIGHT 84.314

MgCO<sub>3</sub>: Crystals 298.15 to 1000 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	65.09	65.09	76.09	-118.280 *	-65.914 *	11.547
UNCERTAINTY		0.14	0.14		1.300	1.340	
400	21.400	89.67	68.27	90.57	-117.810 *	-48.077 *	6.278
500	36.206	110.94	74.73	99.92	-116.976 *	-30.736 *	3.211
600	47.463	129.83	82.37	107.38	-115.850 *	-13.592 *	1.183
700	56.500	146.89	90.39	113.96	-114.434 *	3.343 *	-0.250
800	64.067	162.51	98.44	120.06	-112.711 *	20.050 *	-1.309
900	70.611	176.99	106.38	125.89	-110.660 *	36.529 *	-2.120
1000	76.426	190.54	114.11	131.54	-108.244 *	52.767 *	-2.756

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	11.631 kJ	MOLAR VOLUME	2.8018 J/bar 28.018 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

HEAT CAPACITY EQUATION

$$C_P^0 = 81.119 + 5.2254 \times 10^{-2} T - 1.8320 \times 10^{-4} T^2$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	115	95	220	COMPILED 7-29-76
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## RHODOCHROSITE

FORMULA WEIGHT 114.947

MnCO<sub>3</sub>: Crystals 298.15 to 700 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>p</sub> <sup>o</sup> J/mol·K			
298.15	0.000	100.00	100.00	75.52	-889.270	-816.047	142.969
UNCERTAINTY		2.10	2.10		1.213	1.381	0.242
400	22.250	125.52	103.27	96.10	-888.728	-791.118	103.310
500	38.026	148.06	110.03	105.21	-887.472	-766.862	80.114
600	49.663	167.71	118.05	110.02	-886.120	-742.867	64.673
700	58.503	184.90	126.40	112.81	-884.891	-719.096	53.660

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	kJ	MOLAR VOLUME	3.1073 J/bar 31.073 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.

## HEAT CAPACITY EQUATION

$$C_p^o = 1.2339 \times 10^2 - 2.9399 \times 10^{-3} T - 4.1777 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 700 K)

REFERENCE	168	214	220	COMPILED
		220	68	6- 2-76

STRONTIANITE

FORMULA WEIGHT 147.629

SrCO<sub>3</sub>: Orthorhombic crystals 298.15 to 1197 K. Hexagonal crystals 1197 to 1500 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>p</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	97.07	97.07	81.42	-1218.680	-1137.640	199.311
UNCERTAINTY		1.67	1.67		1.450	1.460	0.256
400	23.375	123.93	100.55	98.06	-1217.718	-1110.080	144.962
500	38.838	146.38	107.54	102.71	-1216.508	-1083.318	113.174
600	49.742	165.38	115.64	105.81	-1215.515	-1056.770	92.000
700	57.996	181.95	123.95	109.35	-1214.727	-1030.390	76.889
800	64.680	196.83	132.15	113.71	-1214.046	-1004.099	65.561
900	70.411	210.51	140.10	118.87	-1214.057	-977.816	56.751
1000	75.541	223.33	147.79	124.72	-1212.958	-951.628	49.708
1100	80.301	235.52	155.22	131.16	-1219.436	-925.109	43.930
1197	84.980	247.34	162.36	137.88	-1216.800	-899.446	39.250
1197	100.703	263.06	162.36	144.77	-1197.976	-899.446	39.250
1200	100.814	263.41	162.60	144.77	-1197.877	-898.688	39.119
1300	104.211	275.02	170.81	144.77	-1194.568	-873.898	35.114
1400	107.121	285.76	178.64	144.77	-1191.346	-849.354	31.690
1500	109.645	295.76	186.11	144.77	-1188.196	-825.031	28.730

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	3.9010 J/bar 39.010 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

STRONTIUM.. ALPHA-GAMMA 828, H. P. GAMMA 1041, B. P. 1652 K.

HEAT CAPACITY EQUATION

$$C_p^0 = - 81.596 + 0.10754 T + 3.1677 \times 10^{-5} T^2 - 1.3914 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1197 K)

REFERENCE	155	120	4	COMPILED 6-29-76
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## STRONTIANITE

FORMULA WEIGHT 147.629

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 SrCO<sub>3</sub>: Orthorhombic crystals 298.15 to 1197 K. Hexagonal crystals 1197 to  
 1500 K.  
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TEMP. K					FORMATION FROM THE OXIDES GIBBS		
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	97.07	97.07	81.42	-234.680 *	-182.917 *	32.045
UNCERTAINTY		1.67	1.67		1.110	1.120	
400	23.375	123.93	100.55	98.06	-234.120 *	-165.839 *	21.656
500	38.838	146.38	107.54	102.71	-233.314 *	-148.864 *	15.552
600	49.742	165.38	115.64	105.81	-232.626 *	-132.048 *	11.496
700	57.996	181.95	123.95	109.35	-231.993 *	-115.337 *	8.606
800	64.680	196.83	132.15	113.71	-231.281 *	-98.712 *	6.445
900	70.411	210.51	140.10	118.87	-230.360 *	-82.200 *	4.771
1000	75.541	223.33	147.79	124.72	-229.117 *	-65.796 *	3.437
1100	80.301	235.52	155.22	131.16	-227.460 *	-49.546 *	2.353
1197	84.980	247.34	162.36	137.88	-225.041 *	-34.142 *	1.490
1197	100.703	263.06	162.36	144.77	-206.218 *	-34.142 *	1.490
1200	100.814	263.41	162.60	144.77	-206.127 *	-33.698 *	1.467
1300	104.211	275.02	170.81	144.77	-203.104 *	-19.464 *	0.782
1400	107.121	285.76	178.64	144.77	-200.230 *	-5.433 *	0.203
1500	109.645	295.76	186.11	144.77	-197.489 *	8.387 *	-0.292

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.9010 J/dar 39.010 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE OXIDES			

## HEAT CAPACITY EQUATION

$$C_P^0 = - 81.596 + 0.10754 T + 3.1677 \times 10^{-3} T^{0.5} - 1.3914 \times 10^{-9} T^{-3}$$

(EQUATION VALID FROM 298 - 1197 K)

REFERENCE	155	120	4	COMPILED 6-29-76
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NITROBARITE

FORMULA WEIGHT 261.350

Ba(NO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to melting point 865 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	213.80	213.80	151.38	-992.070	-796.579	139.558
UNCERTAINTY		0.84	0.84		2.100	2.500	0.438
400	41.700	261.76	220.06	174.97	-990.496	-729.996	95.328
500	70.272	302.86	232.59	193.70	-987.983	-665.149	69.488
600	92.275	339.70	247.42	210.70	-984.858	-600.848	52.309
700	110.357	373.40	263.04	226.90	-979.605	-537.259	40.091
800	125.914	404.73	278.82	242.67	-973.561	-474.459	30.979

MELTING POINT	865	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	8.0580 J/bar 80.580 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

BARIUM..... ALPHA-BETA 582, BETA-GAMMA 768, M. P. GAMMA 1002,  
B. P. 2169 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.2554 \times 10^2 + 0.14967 T - 1.6697 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 800 K)

REFERENCE	238	214	214	COMPILED 6-28-76
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## CALCIUM NITRATE

FORMULA WEIGHT 164.090

Ca(NO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to 800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	193.30	193.30	149.37	-938.390	-742.985	130.168
UNCERTAINTY		0.40	0.40		1.510	1.760	0.308
400	41.350	240.84	199.49	173.81	-936.506	-676.458	88.337
500	69.766	281.70	211.93	192.72	-932.983	-611.833	63.918
600	91.720	318.39	226.67	210.10	-928.173	-548.031	47.711
700	109.833	352.04	242.21	226.88	-922.205	-485.139	36.202
800	125.497	383.41	257.91	243.38	-915.843	-423.083	27.625

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	KJ	MOLAR VOLUME	6.6090 J/bar 66.090 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, H. P. BETA 1112, B. P. 1755 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 1.1481 \times 10^2 + 0.16160 T - 3.6099 \times 10^{-4} T^2$$

(EQUATION VALID FROM 298 - 800 K)

REFERENCE	238	214	214	COMPILED 6-28-76
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NITER FORMULA WEIGHT 101.103

$KNO_3$ : Orthorhombic crystals 298.15 to 401 K. Rhombohedral crystals 401 to melting point 610 K. Liquid 610 to 700 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K			
298.15	0.000	133.09	133.09	96.27	-494.460	-394.544	69.123
UNCERTAINTY		0.67	0.67		0.420	0.420	0.074
400	26.045	163.09	137.04	108.41	-495.591	-360.141	47.030
401	26.293	163.38	137.09	108.53	-495.458	-359.970	46.891
401	40.901	177.99	137.09	120.50	-489.521	-321.970	46.891
500	56.736	204.68	147.94	120.50	-486.815	-328.061	34.272
600	67.362	226.64	159.28	120.50	-484.043	-296.576	25.819
610	68.384	228.73	160.35	120.50	-483.799	-293.450	25.128
610	84.935	245.28	160.35	123.43	-473.703	-293.450	25.128
700	89.734	262.08	172.35	123.43	-471.048	-267.000	19.924

MELTING POINT	610 K	BOILING POINT	K
ENTHALPY OF MELTING	10.096 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.8040 J/bar 48.040 $cm^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

REFERENCE	115	120	215	COMPILED
		215		7-24-76

## MAGNESIUM NITRATE

FORMULA WEIGHT 148.315

Mg(NO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to 600 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	164.01	164.01	141.92	-790.650	-589.181	103.222
UNCERTAINTY		1.60	1.60		1.300	1.420	0.249
400	39.525	209.45	169.92	168.77	-789.474	-520.478	67.968
500	68.066	249.99	181.92	195.63	-786.052	-453.577	47.385
600	91.580	288.05	196.47	222.70	-780.405	-387.573	33.741

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	KJ	MOLAR VOLUME	6.2930 J/bar 62.930 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 58.417 + 27.292 T + 1.8949 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 600 K)

REFERENCE	238	214	214	COMPILED 6-28-76
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AMMONIA-NITER

FORMULA WEIGHT 80.043

NH<sub>4</sub>NO<sub>3</sub>: Ammonia-niter undergoes phase changes at 305.3, 357.4, 398.4 K. It melts at 442.8 K.

TEMP. K					FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	151.08	151.08	139.37	-365.560	-183.803	32.202
UNCERTAINTY		0.21	0.21		0.837	0.879	0.154
400	51.255	208.94	157.69	190.79	-358.483	-122.292	15.970
500	86.692	260.24	173.55	161.08	-349.018	-64.508	6.739

MELTING POINT	442.80 K	BOILING POINT	K
ENTHALPY OF MELTING	5.439 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.6490 J/bar 46.490 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

REFERENCE	115	262	262	COMPILED 7-24-76
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SODA NITER

FORMULA WEIGHT 84.995

NaNO<sub>3</sub>: Alpha crystals 298.15 to 549.2 K. Beta crystals 549.2 to 583.2 K.

Liquid 583.2 to 700 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	116.52	116.52	93.05	-468.020	-367.153	64.324
UNCERTAINTY		0.68	0.68		0.420	0.420	0.074
400	26.097	146.48	120.38	115.76	-469.273	-332.651	43.440
500	46.652	175.14	128.49	138.07	-465.552	-298.883	31.224
600	94.823	234.63	139.81	154.81	-441.240	-266.811	23.228
700	103.393	258.48	155.09	154.81	-435.118	-238.210	17.776

MELTING POINT	583.20 K	BOILING POINT	K
ENTHALPY OF MELTING	15.447 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.7600 J/bar 37.600 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

REFERENCE	115	120 215	215	COMPILED 7-24-76
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STRONTIUM NITRATE

FORMULA WEIGHT 211.630

Sr(NO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to 900 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	194.56	194.56	149.91	-978.220	-779.086	136.493
UNCERTAINTY		0.50	0.50		1.000	1.300	0.228
400	39.975	240.55	200.57	169.18	-977.073	-711.189	92.872
500	68.722	281.42	212.70	197.80	-973.755	-645.055	67.389
600	92.218	319.59	227.37	220.31	-968.370	-579.786	50.475
700	111.644	354.74	243.10	234.84	-961.675	-515.551	38.471
800	127.569	386.65	259.08	242.19	-954.431	-452.311	29.533
900	140.422	415.31	274.89	243.52	-947.983	-389.893	22.629

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	28.677 kJ	MOLAR VOLUME	7.0930 J/bar 70.930 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

STRONTIUM.. ALPHA-GAMMA 828, N. P. GAMMA 1041, B. P. 1652 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.3389 \times 10^3 - 0.37901 T - 2.3582 \times 10^{-4} T^{-0.5} + 2.5757 \times 10^{-7} T^{-2}$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	250	214	214	COMPILED 5-28-76
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## ALUMINUM SULFATE

FORMULA WEIGHT 342.137

Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>: Crystals 298.15 to 1100 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	S <sub>T</sub> <sup>0</sup>	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	C <sub>P</sub> <sup>0</sup>	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	239.32	239.32	259.41	-3440.840	-3099.852	543.084
UNCERTAINTY		1.20	1.20		1.800	1.880	0.329
400	74.850	325.26	250.41	319.87	-3448.086	-2982.237	389.442
500	127.184	400.24	273.06	351.02	-3449.833	-2865.400	299.348
600	166.443	466.31	299.87	373.64	-3448.797	-2748.710	239.298
700	197.447	525.38	327.93	392.95	-3445.683	-2632.212	196.419
800	223.007	579.03	356.02	410.74	-3605.003	-2532.944	165.385
900	244.267	634.22	389.95	401.30	-3595.808	-2405.081	139.588
1000	259.972	676.50	416.53	401.30	-3609.981	-2271.629	118.658
1100	272.820	714.75	441.93	401.30	-3602.799	-2138.165	101.533

## MELTING POINT

K

## BOILING POINT

K

## ENTHALPY OF MELTING

kJ

## ENTHALPY OF VAPORIZATION

kJ

H<sub>298</sub><sup>0</sup> - H<sub>0</sub><sup>0</sup>

kJ

## MOLAR VOLUME

J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.8769 \times 10^2 + 0.15871 T - 2.0037 \times 10^{-6} T^{-3}$$

(EQUATION VALID FROM 298 - 850 K)

REFERENCE 239

262

262

COMPILED

6-29-76

BARITE

FORMULA WEIGHT 233.398

BaSO<sub>4</sub>: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	132.21	132.21	101.75	-1473.190	-1362.186	238.650
UNCERTAINTY		0.84	0.84		1.000	1.300	0.228
400	28.475	164.94	136.46	119.28	-1475.567	-1323.916	172.886
500	47.506	192.50	144.99	127.17	-1477.073	-1285.793	134.326
600	61.172	216.10	154.93	131.46	-1478.672	-1247.418	108.598
700	71.411	236.57	165.16	134.04	-1479.044	-1208.840	90.205
800	79.352	254.59	175.24	135.72	-1534.379	-1175.734	76.768
900	85.678	270.65	184.97	136.87	-1533.286	-1130.916	65.637
1000	90.845	285.11	194.26	137.69	-1532.216	-1086.259	56.741
1100	95.132	298.26	203.13	138.30	-1539.558	-1040.897	49.428
1200	98.750	310.32	211.57	138.76	-1538.802	-995.598	43.337
1300	101.842	321.44	219.60	139.13	-1537.985	-950.357	38.186

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.2100 J/bar 52.100 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

- BARIUM..... ALPHA-BETA 582, BETA-GAMMA 768, H. P. GAMMA 1002,  
B. P. 2169 K.
- SULFUR..... ORTHO-MONO 368.54, H. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.4120 \times 10^2 - 3.5066 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE 115 120 214 COMPILED 7-29-76

## ANHYDRITE

FORMULA WEIGHT 136.138

CaSO<sub>4</sub>: Crystals 298.15 to 1400 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	106.69	106.69	99.66	-1434.110	-1321.696	231.557
UNCERTAINTY		1.67	1.67		4.226	4.184	0.733
400	26.750	137.47	110.72	110.26	-1436.727	-1282.908	167.531
500	44.450	163.16	118.71	120.30	-1437.948	-1244.262	129.988
600	57.920	185.97	128.05	130.21	-1438.205	-1205.527	104.951
700	68.949	206.78	137.83	140.04	-1437.601	-1166.775	87.066
800	78.449	226.12	147.67	149.84	-1491.651	-1133.629	74.019
900	86.922	244.33	157.41	159.62	-1488.282	-1089.009	63.205
1000	94.683	261.66	166.98	169.39	-1484.470	-1044.846	54.577
1100	101.917	278.26	176.34	179.15	-1480.207	-1001.097	47.538
1200	108.759	294.27	185.51	188.90	-1482.418	-957.125	41.663
1300	115.299	309.77	194.47	198.65	-1475.005	-913.642	36.711
1400	121.600	324.85	203.25	208.39	-1466.695	-870.782	32.489

MELTING POINT	1723	K	BOILING POINT	K
ENTHALPY OF MELTING	28.033	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>		kJ	MOLAR VOLUME	4.5940 J/bar 45.940 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 72.182 + 9.7343 \times 10^{-2} T - 1.3733 \times 10^{-5} T^2$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	115	120	214	COMPILED
		214		7-27-76

FERRIC SULFATE

FORMULA WEIGHT 399.867

Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>: Crystals 298.15 to 800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	282.84	282.84	275.01	-2576.930	-2249.555	394.114
UNCERTAINTY		0.85	0.85		2.930	3.010	0.527
400	76.175	370.45	294.27	319.69	-2583.862	-2136.699	279.025
500	128.144	445.29	317.15	351.28	-2586.067	-2024.444	211.493
600	167.683	511.83	344.15	379.15	-2585.415	-1912.270	166.479
700	199.790	572.27	372.48	405.58	-2582.307	-1800.298	134.340
800	227.129	628.11	400.98	431.35	-2741.246	-1705.547	111.361

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	13.0770 J/bar 130.770 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.  
SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.3359 \times 10^2 + 0.24933 T - 8.7230 \times 10^{-6} T^3$$

(EQUATION VALID FROM 298 - 800 K)

REFERENCE	212	212	14	COMPILED 6-28-76
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## ARCANITE

FORMULA WEIGHT 174.254

$K_2SO_4$ : Orthorhombic crystals (alpha) 298.15 to 856 K. Hexagonal crystals  
(beta) 856 to melting point 1342 K. Liquid 1342 to 1700 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	175.56	175.56	130.04	-1437.700	-1319.662	231.200
UNCERTAINTY		0.35	0.35		0.540	0.540	0.095
400	35.667	216.65	180.98	149.06	-1445.193	-1278.057	166.898
500	59.832	251.50	191.67	163.03	-1445.817	-1236.116	129.137
600	77.543	281.75	204.21	175.17	-1445.207	-1194.265	103.970
700	91.989	309.24	217.25	186.44	-1443.170	-1152.547	86.004
800	105.122	335.56	230.43	197.25	-1493.925	-1116.844	72.923
856	111.137	350.29	239.02	203.18	-1490.991	-1090.949	66.572
856	121.868	360.89	239.02	218.98	-1481.805	-1090.949	66.572
900	125.422	369.92	244.50	203.55	-1479.752	-1070.920	62.155
1000	132.337	390.44	258.10	189.91	-1475.086	-1025.762	53.581
1100	137.791	408.76	270.97	197.63	-1629.289	-972.403	46.176
1200	143.621	426.82	283.20	219.88	-1621.631	-913.004	39.742
1300	150.682	445.65	294.97	252.38	-1611.284	-854.352	34.328
1342	151.000	450.81	299.81	268.37	-1610.064	-828.710	32.256
1342	179.247	479.06	299.81	197.61	-1572.157	-828.710	32.256
1400	180.007	486.97	306.96	197.61	-1568.429	-797.351	29.750
1500	181.180	500.61	319.43	197.61	-1562.002	-742.510	25.857
1600	182.207	513.36	331.15	197.61	-1555.627	-688.093	22.464
1700	183.114	525.34	342.23	197.61	-1549.301	-634.058	19.482

MELTING POINT	1342	K	BOILING POINT	K
ENTHALPY OF MELTING	37.907	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	6.5500 J/bar 65.500 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. H. P. 336.4, B. P. 1030 K.

SULFUR..... ORTHO-MONO 368.54, H. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 120.37 + 9.9579 \times 10^{-2} T - 1.7824 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 856 K)

$$C_P^0 = -8.4452 \times 10^{-2} + 0.68449 T + 3.4994 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 856 - 1342 K)

REFERENCE	239	215	215	COMPILED 6-28-76
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POTASSIUM ALUMINUM SULFATE

FORMULA WEIGHT 258.195

KAl(SO<sub>4</sub>)<sub>2</sub>: Crystals 298.15 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	204.60	204.60	192.97	-2470.150	-2239.790	392.404
UNCERTAINTY		1.26	1.26		1.300	1.380	0.242
400	54.525	267.25	212.73	230.89	-2477.813	-2159.839	282.047
500	92.070	321.22	229.15	252.19	-2479.424	-2080.032	217.300
600	120.073	368.60	248.53	267.34	-2479.034	-2000.262	174.139
700	142.010	410.76	268.75	279.58	-2477.202	-1920.570	143.315
800	159.885	448.80	288.92	290.27	-2583.688	-1852.324	120.945
900	174.922	483.56	308.64	300.06	-2577.590	-1761.151	102.215
1000	187.901	515.66	327.76	309.30	-2581.667	-1670.019	87.233

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	9.2330 J/bar 92.330 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

ALUMINUM... M. P. 933 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.3700 \times 10^2 + 7.8284 \times 10^{-2} T - 5.9884 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	265	265	265	COMPILED 6-28-76
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## ALUNITE

FORMULA WEIGHT 828.406

K<sub>2</sub>Al<sub>6</sub>(OH)<sub>12</sub>(SO<sub>4</sub>)<sub>6</sub>: Crystals 298.15 to 700 K.

TEMP. K					FORMATION FROM THE ELEMENTS GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	656.05	656.05	745.17	---	---	---
UNCERTAINTY		3.77	3.77				
400	216.150	904.24	688.09	925.89	---	---	---
500	367.720	1121.21	753.49	1014.98	---	---	---
600	481.010	1312.01	831.00	1077.37	---	---	---
700	569.996	1482.08	912.08	1129.36	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	29.3600 J/bar 293.600 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

ALUMINUM... M. P. 933 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 8.5901 \times 10^2 + 0.41235 T - 6.2756 \times 10^{-3} T^{-3}$$

(EQUATION VALID FROM 298 - 700 K)

REFERENCE 121 120

COMPILED  
6-29-76

MANGANESE SULFATE

FORMULA WEIGHT 150.996

MnSO<sub>4</sub>: Crystals 298.15 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	112.13	112.13	100.50	-1065.250	-957.326	167.720
UNCERTAINTY		0.85	0.85		1.050	1.300	0.228
400	28.175	144.50	116.32	118.66	-1067.454	-920.119	120.156
500	47.368	172.17	124.80	129.00	-1068.017	-883.166	92.264
600	61.620	196.38	134.76	136.45	-1067.759	-846.259	73.674
700	72.754	217.88	145.13	142.52	-1066.914	-809.388	60.398
800	81.815	237.27	155.46	147.87	-1120.316	-778.230	50.813
900	89.433	254.97	165.54	152.79	-1117.466	-735.572	42.692
1000	96.002	271.31	175.31	157.45	-1116.615	-693.261	36.212

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.3620 J/bar 43.620 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.  
SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.2028 \times 10^{-2} + 3.9993 \times 10^{-5} T - 2.8181 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	242	263	263	COMPILED 6- 8-76
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## BASCAGNITE

FORMULA WEIGHT 132.134

(NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>: Crystals 298.15 to 600 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	220.08	220.08	187.49	-1180.850	-901.677	157.971
UNCERTAINTY		1.25	1.25		1.255	1.339	0.235
400	51.350	279.15	227.80	215.88	-1185.821	-805.519	105.190
500	87.048	330.31	243.26	243.76	-1187.521	-710.150	74.189
600	115.488	377.22	261.73	271.64	-1186.375	-614.781	53.522

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	7.4680 J/bar 74.680 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE ELEMENTS			

## HEAT CAPACITY EQUATION

$$C_p^0 = 1.0438 \times 10^2 + 0.27876 T$$

(EQUATION VALID FROM 298 - 600 K)

REFERENCE	121	120	262	COMPILED
	239	262		6-28-76

AMMONIUM BISULFATE

FORMULA WEIGHT 115.104

NH<sub>4</sub>HSO<sub>4</sub>: Crystals 298.15 to melting point 417 K. Liquid 417 to 600 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$\frac{S_T^0}{S_{298}^0} - (G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $f$
298.15	0.000	0.00	---	142.88	---	---
UNCERTAINTY						
400	40.792	46.86	---	177.40	---	---
417	46.355	54.22	---	183.16	---	---
417	80.670	88.53	---	197.12	---	---
500	102.192	126.64	---	223.63	---	---
600	125.093	170.24	---	255.57	---	---

MELTING POINT	417 K	BOILING POINT	K
ENTHALPY OF MELTING	14.310 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	6.5070 J/bar 65.070 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 63.922 + 0.31941 T$$

(EQUATION VALID FROM 417 - 600 K)

REFERENCE 239

COMPILED  
6-28-76

## THEBARDITE

FORMULA WEIGHT 142.037

$\text{Ba}_2\text{SO}_4$ : Orthorhombic crystals (V) 298.15 to 450 K. Orthorhombic crystals (III) 450 to 514 K. Hexagonal crystals (I) 514 to 1155 K. Liquid 1155 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K			
298.15	0.000	149.58	149.58	127.28	-1387.790	-1269.985	222.497
UNCERTAINTY		0.08	0.08		0.420	0.420	0.074
400	36.807	191.96	155.16	146.82	-1395.113	-1229.048	160.498
450	49.929	210.10	160.17	162.80	-1395.497	-1208.123	140.235
450	56.809	216.98	160.17	164.77	-1392.401	-1208.123	140.235
500	68.032	234.89	166.86	173.30	-1392.077	-1187.782	124.087
514	70.981	239.66	168.68	176.40	-1392.002	-1182.022	120.122
514	84.651	253.34	168.68	163.78	-1384.976	-1182.022	120.122
600	96.290	279.30	183.01	170.78	-1384.277	-1148.353	99.973
700	107.514	306.23	198.72	178.92	-1382.534	-1109.125	82.764
800	116.949	330.66	213.71	187.06	-1434.556	-1075.797	70.243
900	125.189	353.16	227.97	195.20	-1429.852	-1031.172	59.848
1000	132.600	374.15	241.55	203.34	-1424.453	-987.159	51.564
1100	139.402	393.91	254.51	211.48	-1418.395	-943.707	44.813
1155	143.392	404.12	260.72	215.96	-1414.289	-919.498	41.584
1155	163.931	424.65	260.72	196.55	-1390.566	-919.498	41.584
1200	165.140	431.72	266.58	196.37	-1583.206	-896.335	39.017
1300	167.527	447.42	279.89	195.98	-1576.781	-839.366	33.726
1400	169.543	461.93	292.39	195.58	-1570.476	-782.895	29.210
1500	171.267	475.41	304.14	195.19	-1564.269	-726.849	25.311
1600	172.750	487.99	315.24	194.80	-1558.155	-671.219	21.913
1700	174.035	499.79	325.76	194.40	-1552.133	-615.987	18.927
1800	175.155	510.89	335.74	194.01	-1546.200	-561.093	16.283

MELTING POINT	1155 K	BOILING POINT	K
ENTHALPY OF MELTING	23.723 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.3330 J/bar 53.330 $\text{cm}^3$

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... H. P. 370.98, B. P. 1175 K.

SULFUR..... ORTHO-HOMO 368.54, H. P. HOMO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.2193 \times 10^2 + 8.1413 \times 10^{-2} T$$

(EQUATION VALID FROM 514 - 1155 K)

$$C_P^0 = 2.0110 \times 10^2 - 3.9406 \times 10^{-3} T$$

(EQUATION VALID FROM 1155 - 1800 K)

REFERENCE	42	215	215	COMPILED
				6-28-76

ANGLSITE

FORMULA WEIGHT 303.258

PbSO<sub>4</sub>: Crystals 298.15 to 1100 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	148.57	148.57	104.31	-919.940	-813.026	142.439
UNCERTAINTY		0.29	0.29		1.088	1.046	0.183
400	26.950	179.65	152.70	108.70	-922.605	-776.138	101.354
500	44.154	204.82	160.67	117.60	-924.147	-739.286	77.233
600	57.267	227.18	169.91	128.27	-924.675	-702.287	61.140
700	68.224	247.81	179.59	139.77	-928.962	-664.443	49.582
800	77.911	267.25	189.34	151.72	-981.914	-632.308	41.286
900	86.789	285.82	199.03	163.93	-977.749	-588.781	34.172
1000	95.119	303.73	208.61	176.30	-972.448	-545.834	28.512
1100	103.065	321.12	218.05	188.78	-965.983	-503.494	23.909

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	20.062 kJ	MOLAR VOLUME	4.7950 J/bar 47.950 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LEAD..... M. P. 600.6, B. P. 2021 K.

SULFUR..... ORTHO-RHOMBO 368.54, M. P. RHOMBO 388.36,  
B. P. 716.9 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 46.827 + 0.12775 T + 1.7241 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1100 K)

REFERENCE	115	262	262	COMPILED 7-27-76
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## ZINKOSITE

FORMULA WEIGHT 161.438

ZnSO<sub>4</sub>: Crystals 298.15 to 1000 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	110.46	110.46	104.13	-982.820	-871.530	152.689
UNCERTAINTY		1.25	1.25		0.837	0.962	0.169
400	26.375	140.90	114.52	104.85	-985.596	-833.141	108.797
500	42.722	164.99	122.27	111.90	-987.518	-794.747	83.027
600	55.022	186.21	131.19	121.41	-988.579	-756.123	65.827
700	65.259	205.71	140.45	132.09	-996.002	-717.266	53.523
800	74.312	224.08	149.77	143.38	-1049.874	-683.036	44.598
900	82.633	241.64	159.01	155.02	-1046.723	-637.307	36.988
1000	90.461	258.59	168.13	166.90	-1042.527	-592.033	30.925

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.1570 J/bar 41.570 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

ZINC..... M. P. 692.7, B. P. 1178 K.

SULFUR..... ORTHO-MONO 368.54, M. P. MONO 388.36,  
B. P. 716.9 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 40.186 + 0.12432 T + 2.3892 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	115	271	262	COMPILED
			3	7-29-76



BERLINITE

FORMULA WEIGHT 121.953

AlPO<sub>4</sub>: Crystals 298.15 to 800 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	90.79	90.79	93.18	-1716.400	-1605.875	281.344
UNCERTAINTY		0.21	0.21		2.092	2.134	0.374
400	26.025	120.71	94.69	110.97	-1716.857	-1568.013	204.763
500	44.324	146.87	102.55	122.97	-1716.242	-1530.855	159.928
600	58.120	170.02	111.90	131.01	-1715.104	-1493.878	130.054
700	69.161	190.88	121.72	140.52	-1713.577	-1457.132	108.733
800	79.005	210.61	131.60	156.82	-1796.663	-1442.815	94.207

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	14.761 kJ	MOLAR VOLUME	4.6580 J/bar 46.580 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... H. P. 933 K.

PHOSPHORUS. SUBLINES 704 K.

HEAT CAPACITY EQUATION

$$C_P^0 = -3.5888 \times 10^3 + 3.1323 \times 10^2 T^{0.5} - 8.2315 T + 1.9776 \times 10^{-3} T^2$$

$$1.6454 \times 10^5 T^{-1}$$

(EQUATION VALID FROM 298 - 830 K)

REFERENCE	151	262	262	COMPILED 03-15-79
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## WHITLOCKITE

FORMULA WEIGHT 310.183

$\text{Ca}_3(\text{PO}_4)_2$ : Rhombohedral crystals 298.15 to 1373 K. Monoclinic crystals 1373 to 1600 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	235.98	235.98	227.82	-4085.925	-3860.760	676.394
UNCERTAINTY		0.84	0.84		2.100	2.200	0.385
400	62.075	307.46	245.38	255.19	-4085.591	-3783.851	494.122
500	102.738	366.59	263.85	275.25	-4084.165	-3708.572	387.434
600	133.072	418.45	285.38	294.10	-4081.949	-3633.634	316.337
700	157.386	465.17	307.78	312.39	-4079.141	-3559.161	265.589
800	177.887	508.06	330.17	330.37	-4248.877	-3529.180	230.433
900	195.822	548.00	352.18	348.17	-4242.604	-3439.542	199.627
1000	211.940	585.60	373.66	365.87	-4236.054	-3350.664	175.021
1100	226.735	621.29	394.56	383.49	-4229.191	-3262.464	154.922
1200	240.529	655.42	414.89	401.06	-4242.840	-3173.049	138.120
1300	253.553	688.21	434.66	418.60	-4228.705	-3084.466	123.936
1373	262.681	711.67	448.99	431.39	-4217.337	-3020.356	114.907
1373	273.956	722.95	448.99	330.54	-4201.857	-3020.356	114.907
1400	274.949	729.27	454.32	330.54	-4200.391	-2997.637	111.844
1500	278.654	752.08	473.42	330.54	-4194.454	-2911.910	101.402
1600	281.897	773.41	491.52	330.54	-4188.637	-2826.637	92.281

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	9.7620 J/bar 97.620 $\text{cm}^3$

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

PHOSPHORUS. SUBLINES 704 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.9285 \times 10^2 + 0.17419 T - 1.1736 \times 10^{-4} T^2$$

(EQUATION VALID FROM 298 - 1373 K)

REFERENCE	115	214	214	COMPILED 03-15-79
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WHITLOCKITE

FORMULA WEIGHT 310.183

Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>: Rhombohedral crystals 298.15 to 1373 K. Monoclinic crystals 1373 to 1600 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	235.98	235.98	227.82	-710.653 *	-712.396 *	124.809
UNCERTAINTY		0.84	0.84				
400	62.075	307.46	245.38	255.19	-712.004 *	-712.832 *	93.086
500	102.738	366.59	263.85	275.25	-714.778 *	-712.745 *	74.460
600	133.072	418.45	285.38	294.10	-718.596 *	-711.990 *	61.984
700	157.386	465.17	307.78	312.39	-723.271 *	-710.543 *	53.021
800	177.887	508.06	330.17	330.37	-728.667 *	-708.363 *	46.251
900	195.822	548.00	352.18	348.17	-734.658 *	-705.466 *	40.944
1000	211.940	585.60	373.66	365.87	-741.176 *	-701.880 *	36.662
1100	226.735	621.29	394.56	383.49	---	---	---
1200	240.529	655.42	414.89	401.06	---	---	---
1300	253.553	688.21	434.66	418.60	---	---	---
1373	262.681	711.67	448.99	431.39	---	---	---
1373	273.956	722.95	448.95	330.54	---	---	---
1400	274.949	729.27	454.32	330.54	---	---	---
1500	278.654	752.08	473.42	330.54	---	---	---
1600	281.897	773.41	491.52	330.54	---	---	---

MELTING POINT

K

BOILING POINT

K

ENTHALPY OF MELTING

kJ

ENTHALPY OF VAPORIZATION

kJ

$H_{298}^0 - H_0^0$

kJ

MOLAR VOLUME

9.7620 J/bar  
97.620 cm<sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

P<sub>2</sub>O<sub>5</sub>..... M. P. 842 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.9285 \times 10^2 + 0.17419 T - 1.1736 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1373 K)

REFERENCE 115

214

214

COMPILED  
7-27-76

## HYDROXYAPATITE

FORMULA WEIGHT 502.321

Ca<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>OH: Crystals 298.15 to 1500 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	390.37	390.37	385.10	-6669.259	-6286.093	1101.302
UNCERTAINTY		1.67	1.67		5.000	5.000	0.876
400	106.900	513.31	406.41	446.35	-6667.545	-6155.325	803.807
500	178.142	616.52	438.38	477.23	-6663.244	-6027.762	629.719
600	229.773	705.43	475.66	497.55	-6658.313	-5901.106	513.739
700	269.189	783.35	514.16	513.28	-6653.651	-5775.324	430.962
800	300.561	852.78	552.22	526.80	-6909.611	-5716.202	373.231
900	326.389	915.55	589.16	539.15	-6902.718	-5567.379	323.123
1000	348.259	972.97	624.71	550.89	-6897.107	-5419.322	283.078
1100	367.201	1026.01	658.81	562.29	-6892.774	-5271.788	250.338
1200	383.926	1075.42	691.49	573.50	-6924.440	-5121.478	222.933
1300	398.936	1121.76	722.82	584.61	-6911.624	-4971.763	199.769
1400	412.593	1165.49	752.90	595.67	-6897.959	-4823.090	179.952
1500	425.167	1206.97	781.80	606.72	-6883.402	-4675.360	162.811

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	64.245 kJ	MOLAR VOLUME	15.9600 J/bar 159.600 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

PHOSPHORUS. SUBLIMES 704 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 3.8776 \times 10^{-2} + 0.11856 T + 1.8112 \times 10^{-5} T^2 - 1.2703 \times 10^{-7} T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	52	120	214 150	COMPILED 03-15-79
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FLUORAPATITE

FORMULA WEIGHT 504.313

Ca<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>F: Crystals 298.15 to 1600 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	387.86	387.86	375.93	-6819.860	-6455.778	1131.033
UNCERTAINTY		1.67	1.67		5.000	5.000	0.876
400	102.725	506.04	403.31	426.53	-6818.464	-6331.506	826.813
500	170.858	604.86	434.00	458.27	-6814.827	-6210.185	648.776
600	220.715	690.49	469.77	480.52	-6810.383	-6089.647	530.153
700	259.059	765.85	506.79	496.94	-6806.063	-5969.908	445.482
800	289.611	833.07	543.46	509.49	-7062.361	-5916.800	386.329
900	314.611	893.67	579.06	519.30	-7055.955	-5773.932	335.112
1000	335.482	948.80	613.32	527.09	-7051.144	-5631.760	294.174
1100	353.196	999.34	646.14	533.35	-7048.036	-5490.009	260.700
1200	368.427	1045.97	677.54	538.40	-7081.464	-5345.348	232.678
1300	381.665	1089.23	707.57	542.49	-7071.045	-5201.104	208.984
1400	393.271	1129.56	736.29	545.79	-7060.490	-5057.699	188.706
1500	403.535	1167.31	763.78	548.45	-7049.820	-4914.979	171.155
1600	412.661	1202.78	790.12	550.55	-7039.109	-4773.056	155.825

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
$H_{298}^0 - H_0^0$	63.471 kJ	MOLAR VOLUME	15.7560 J/bar 157.560 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

PHOSPHORUS. SUBLINES 704 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 7.5433 \times 10^{-2} - 3.0255 \times 10^{-2} T - 6.2005 \times 10^{-3} T^{-0.5} - 9.0838 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	52	120	214	COMPILED
				03-15-79

## DICESIUM URANATE

FORMULA WEIGHT 567.837

Cs<sub>2</sub>UO<sub>4</sub>: Crystals 298.15 to 1100 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	219.66	219.66	152.76	-1920.000	-1797.300	314.881
UNCERTAINTY		0.42	0.42		3.500	3.800	0.666
400	40.225	266.01	225.78	162.06	-1925.017	-1753.901	229.037
500	65.142	302.77	237.63	167.28	-1924.351	-1711.186	178.767
600	82.482	333.61	251.13	170.92	-1922.817	-1668.681	145.272
700	95.326	360.17	264.84	173.77	-1921.005	-1626.473	121.369
800	105.284	383.54	278.26	176.17	-1919.439	-1584.503	103.458
900	113.278	404.41	291.13	178.31	-1918.614	-1542.686	89.536
1000	119.883	423.30	303.42	180.27	-2053.313	-1492.575	77.964
1100	125.457	440.57	315.11	182.11	-2055.172	-1436.400	68.209

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	30.815 kJ	MOLAR VOLUME	8.5400 J/bar 85.400 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

CESIUM..... M. P. 301.55, B. P. 942 K.

URANIUM.... ALPHA-BETA 941, BETA-GAMMA 1048, M. P. 1405 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 1.7383 \times 10^2 + 1.3456 \times 10^{-2} T - 1.8078 \times 10^2 T^{-0.5} - 1.2988 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1100 K)

REFERENCE	64	193	185	COMPILED
			89	5-19-76

DISODIUM URANATE (ALPHA)

FORMULA WEIGHT 348.006

Na<sub>2</sub>UO<sub>4</sub>: Crystals 298.15 to 1100 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	166.02	166.02	146.67	-1887.000	-1768.600	309.853
UNCERTAINTY		0.33	0.33		3.000	3.600	0.631
400	39.225	211.19	171.97	159.84	-1891.627	-1727.808	225.629
500	64.124	247.70	183.58	167.11	-1890.668	-1686.968	176.237
600	81.733	278.64	196.91	172.22	-1889.384	-1646.342	143.327
700	94.961	305.50	210.54	176.34	-1887.998	-1605.933	119.837
800	105.362	329.29	223.93	179.93	-1886.648	-1565.736	102.232
900	113.833	350.67	236.84	183.23	-1885.452	-1525.687	88.549
1000	120.929	370.14	249.21	186.35	-1886.911	-1485.611	77.601
1100	127.014	388.04	261.03	189.35	-1889.764	-1445.310	68.632

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	26.227 kJ	MOLAR VOLUME	5.8500 J/bar 58.500 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

URANIUM.... ALPHA-BETA 941, BETA-GAMMA 1048, M. P. 1405 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.5846 \times 10^2 + 2.7434 \times 10^{-2} T + 84.123 T^{-0.5} - 2.2082 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1165 K)

REFERENCE	64	195	89	COMPILED
			184	5-19-76

## TRISODIUM URANIUM OXIDE

FORMULA WEIGHT 370.996

Na<sub>3</sub>UO<sub>4</sub>: Crystals 298.15 to 1200 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	198.20	198.20	173.01	-2021.500	-1897.400	332.418
UNCERTAINTY		0.40	0.40		4.000	4.200	0.736
400	46.100	251.32	205.22	187.01	-2029.052	-1854.425	242.164
500	74.996	293.81	218.81	193.46	-2028.509	-1810.829	189.177
600	95.115	329.48	234.36	197.78	-2027.648	-1767.368	153.864
700	110.046	360.24	250.19	201.42	-2026.683	-1724.045	128.650
800	121.686	387.37	265.68	204.92	-2025.742	-1680.885	109.751
900	131.133	411.71	280.58	208.44	-2024.923	-1637.824	95.057
1000	139.042	433.86	294.82	212.08	-2026.726	-1594.696	83.299
1100	145.851	454.24	308.39	215.83	-2029.880	-1551.293	73.665
1200	151.844	473.19	321.35	219.72	-2320.051	-1501.720	65.368

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	31.109 kJ	MOLAR VOLUME	J/bar

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

URANIUM.... ALPHA-BETA 941, BETA-GAMMA 1048, M. P. 1405 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.1152 \times 10^2 + 5.3894 \times 10^{-2} T + 1.6100 \times 10^3 T^{-0.5} - 4.2510 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1212.70 K)

REFERENCE	62	194	89	COMPILED
			186	6- 8-76



KYANITE

FORMULA WEIGHT 162.047

Al<sub>2</sub>SiO<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS							
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>	
298.15	0.000	83.76	83.76	121.70	-2591.730	-2441.276	427.703	
UNCERTAINTY		0.34	0.34		1.900	1.920	0.336	
400	34.825	123.76	88.94	149.24	-2592.612	-2389.682	312.062	
500	59.438	158.92	99.48	165.27	-2592.009	-2339.004	244.355	
600	77.995	190.03	112.04	175.60	-2590.697	-2288.516	199.234	
700	92.476	217.66	125.18	182.71	-2589.084	-2238.279	167.023	
800	104.096	242.42	138.32	187.94	-2587.414	-2188.275	142.880	
900	113.656	264.80	151.14	192.11	-2585.835	-2138.464	124.114	
1000	121.680	285.23	163.55	195.72	-2605.752	-2087.312	109.030	
1100	128.566	304.05	175.48	199.13	-2603.794	-2035.566	96.661	
1200	134.589	321.52	186.93	202.59	-2601.638	-1983.993	86.361	
1300	139.959	337.88	197.92	206.26	-2599.246	-1932.606	77.653	
1400	144.836	353.31	208.47	210.28	-2596.584	-1881.451	70.198	
1500	149.345	367.97	218.63	214.76	-2593.592	-1830.465	63.743	

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	16.041 kJ	MOLAR VOLUME	4.4090 J/bar 44.090 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 4.3612 \times 10^{-5} T^2 - 0.13576 T + 4.7236 \times 10^{-5} T^2 - 4.8027 \times 10^{-8} T^{-0.5}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	205	120	99	COMPILED
			98	7- 8-76

## KYANITE

FORMULA WEIGHT 162.047

Al<sub>2</sub>SiO<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	83.76	83.76	121.70	-5.330 *	-2.760 *	0.484
UNCERTAINTY		0.34	0.34		0.960	0.970	
400	34.825	123.76	88.94	149.24	-5.460 *	-1.860 *	0.243
500	59.438	158.92	99.48	165.27	-5.485 *	-0.955 *	0.100
600	77.995	190.03	112.04	175.60	-5.536 *	-0.040 *	0.004
700	92.476	217.66	125.18	182.71	-5.728 *	0.887 *	-0.066
800	104.096	242.42	138.32	187.94	-6.138 *	1.854 *	-0.121
900	113.656	264.80	151.14	192.11	-6.710 *	2.902 *	-0.168
1000	121.680	285.23	163.55	195.72	-6.552 *	3.958 *	-0.207
1100	128.566	304.05	175.48	199.13	-6.343 *	4.986 *	-0.237
1200	134.589	321.52	186.93	202.59	-6.066 *	6.017 *	-0.262
1300	139.959	337.88	197.92	206.26	-5.681 *	7.007 *	-0.282
1400	144.836	353.31	208.47	210.28	-5.140 *	7.964 *	-0.297
1500	149.345	367.97	218.63	214.76	-4.399 *	8.861 *	-0.309

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	16.041 kJ	MOLAR VOLUME	4.4090 J/bar 44.090 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 4.3612 \times 10^{-2} - 0.13576 T + 4.7236 \times 10^{-5} T^2 - 4.8027 \times 10^{-8} T^{-0.5}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	205	120	99	COMPILED
			98	7- 8-76

ANDALUSITE

FORMULA WEIGHT 162.047

Al<sub>2</sub>SiO<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	93.22	93.22	122.70	-2587.525	-2439.892	427.458
UNCERTAINTY		0.42	0.42		2.100	2.100	0.368
400	34.900	133.31	98.41	148.98	-2588.377	-2389.267	312.005
500	59.384	168.35	108.97	164.49	-2587.831	-2339.541	244.409
600	77.800	199.29	121.49	174.61	-2586.609	-2289.984	199.360
700	92.157	226.77	134.61	181.61	-2585.102	-2240.674	167.201
800	103.675	251.37	147.69	186.74	-2583.546	-2191.567	143.094
900	113.133	273.60	160.47	190.73	-2582.100	-2142.649	124.356
1000	121.063	293.87	172.81	194.06	-2602.164	-2092.364	109.294
1100	127.835	312.51	184.67	197.05	-2600.393	-2041.471	96.941
1200	133.723	329.78	196.06	199.93	-2598.472	-1990.739	86.654
1300	138.928	345.90	206.97	202.86	-2596.362	-1940.168	77.957
1400	143.607	361.04	217.43	205.96	-2594.099	-1889.788	70.509
1500	147.871	375.36	227.49	209.33	-2591.597	-1839.555	64.059
1600	151.826	388.99	237.16	213.03	-2588.828	-1789.522	58.422

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	17.096 kJ	MOLAR VOLUME	5.1530 J/bar 51.530 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 4.0843 \times 10^2 - 0.11050 T + 3.5897 \times 10^{-5} T^2 - 4.4199 \times 10^3 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	205	120	285 267	COMPILED 10-12-77
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ANDALUSITE FORMULA WEIGHT 162.047

Al<sub>2</sub>SiO<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY	FREE ENERGY	Log $K_f$
					kJ/mol	kJ/mol	
298.15	0.000	93.22	93.22	122.70	-1.125 *	-1.376 *	0.241
UNCERTAINTY		0.42	0.42		1.260	1.260	0.221
400	34.900	133.31	98.41	148.98	-1.225 *	-1.445 *	0.189
500	59.384	168.35	108.97	164.49	-1.307 *	-1.492 *	0.156
600	77.800	199.29	121.49	174.61	-1.448 *	-1.508 *	0.131
700	92.157	226.77	134.61	181.61	-1.746 *	-1.508 *	0.113
800	103.675	251.37	147.69	186.74	-2.267 *	-1.438 *	0.094
900	113.133	273.60	160.47	190.73	-2.975 *	-1.283 *	0.074
1000	121.063	293.87	172.81	194.06	-2.964 *	-1.094 *	0.057
1100	127.835	312.51	184.67	197.05	-2.942 *	-0.919 *	0.044
1200	133.723	329.78	196.06	199.93	-2.900 *	-0.729 *	0.032
1300	138.928	345.90	206.97	202.86	-2.817 *	-0.555 *	0.022
1400	143.607	361.04	217.43	205.96	-2.655 *	-0.373 *	0.014
1500	147.871	375.36	227.49	209.33	-2.404 *	-0.229 *	0.008
1600	151.826	388.99	237.16	213.03	-1.995 *	-0.090 *	0.003

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	17.096 kJ	MOLAR VOLUME	5.1530 J/bar 51.530 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 4.0843 \times 10^2 - 0.11050 T + 3.5897 \times 10^{-5} T^2 - 4.4199 \times 10^3 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	205	120	285	COMPILED
			267	10-12-77

SILLIMANITE

FORMULA WEIGHT 162.047

Al<sub>2</sub>SiO<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS							
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	S <sub>T</sub> <sup>0</sup>	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	C <sub>P</sub> <sup>0</sup>	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	96.11	96.11	122.60	-2585.760	-2438.988	427.302	
UNCERTAINTY		0.42	0.42		1.740	1.750	0.307	
400	35.025	136.33	101.30	149.06	-2586.562	-2388.660	311.928	
500	59.310	171.20	111.89	162.79	-2586.103	-2339.238	244.380	
600	77.348	201.72	124.37	171.78	-2585.115	-2289.948	199.359	
700	91.339	228.72	137.38	178.53	-2583.910	-2240.847	167.215	
800	102.595	252.94	150.34	184.10	-2582.645	-2191.922	143.118	
900	111.922	274.91	162.99	188.97	-2581.425	-2143.153	124.386	
1000	119.855	295.05	175.19	193.41	-2601.607	-2092.987	109.327	
1100	126.732	313.68	186.95	197.57	-2599.842	-2042.207	96.977	
1200	132.801	331.04	198.24	201.53	-2597.814	-1991.593	86.692	
1300	138.236	347.32	209.08	205.37	-2595.516	-1941.148	77.997	
1400	143.164	362.68	219.52	209.10	-2592.954	-1890.939	70.552	
1500	147.683	377.23	229.55	212.76	-2590.115	-1840.878	64.105	

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	17.414 kJ	MOLAR VOLUME	4.9900 J/bar 49.900 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.6442 \times 10^{-2} + 3.3594 \times 10^{-2} T - 4.6078 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	205	120	31	COMPILED
			267	7- 8-76

## SILLIMANITE

FORMULA WEIGHT 162.047

Al<sub>2</sub>SiO<sub>5</sub>: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	96.11	96.11	122.60	0.640 *	-0.472 *	0.083
UNCERTAINTY		0.42	0.42		0.590	0.600	
400	35.025	136.33	101.30	149.06	0.590 *	-0.838 *	0.109
500	59.310	171.20	111.89	162.79	0.421 *	-1.189 *	0.124
600	77.348	201.72	124.37	171.78	0.046 *	-1.472 *	0.128
700	91.339	228.72	137.38	178.53	-0.554 *	-1.681 *	0.125
800	102.595	252.94	150.34	184.10	-1.369 *	-1.793 *	0.117
900	111.922	274.91	162.99	188.97	-2.300 *	-1.787 *	0.104
1000	119.855	295.05	175.19	193.41	-2.407 *	-1.717 *	0.090
1100	126.732	313.68	186.95	197.57	-2.391 *	-1.655 *	0.079
1200	132.801	331.04	198.24	201.53	-2.242 *	-1.583 *	0.069
1300	138.236	347.32	209.08	205.37	-1.951 *	-1.535 *	0.062
1400	143.164	362.68	219.52	209.10	-1.510 *	-1.524 *	0.057
1500	147.683	377.23	229.55	212.76	-0.922 *	-1.552 *	0.054

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	17.414 kJ	MOLAR VOLUME	4.9900 J/bar 49.900 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.6442 \times 10^2 + 3.3594 \times 10^{-4} T - 4.6078 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	205	120	31	COMPILED
			267	7- 8-76

MULLITE (3-2)

FORMULA WEIGHT 426.056

3Al<sub>2</sub>O<sub>3</sub>·2SiO<sub>2</sub>: Crystals 298.15 to melting point 2133 K.

TEMP. K	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>P</sub> <sup>o</sup> J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	269.57	269.57	326.10	-6810.421	-6431.286	1126.739
UNCERTAINTY		4.18	4.18		2.200	2.220	0.389
400	92.275	375.60	283.32	392.41	-6812.769	-6301.260	822.864
500	156.542	467.72	311.18	431.95	-6811.616	-6173.481	644.942
600	204.813	549.00	344.19	458.85	-6808.737	-6046.104	526.362
700	242.569	621.27	378.70	478.36	-6805.066	-5919.294	441.705
800	273.006	686.15	413.14	493.13	-6801.209	-5792.991	378.245
900	298.133	744.93	446.80	504.61	-6797.606	-5667.173	328.916
1000	319.249	798.58	479.33	513.73	-6858.509	-5537.159	289.233
1100	337.275	847.90	510.63	521.06	-6853.935	-5405.233	256.674
1200	352.847	893.50	540.65	527.02	-6849.053	-5273.739	229.561
1300	366.438	935.89	569.45	531.88	-6843.927	-5142.630	206.634
1400	378.400	975.45	597.05	535.85	-6838.642	-5012.022	187.002
1500	389.011	1012.54	623.53	539.09	-6833.221	-4881.717	169.997
1600	398.476	1047.42	648.94	541.73	-6827.734	-4751.816	155.132
1700	406.968	1080.33	673.36	543.85	-6923.211	-4621.451	142.001
1800	414.621	1111.46	696.84	545.53	-6917.091	-4486.139	130.185

MELTING POINT	2133	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>		kJ	MOLAR VOLUME	13.4550 J/bar 134.550 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^o = 7.5455 \times 10^{-2} - 2.9426 \times 10^{-2} T + 6.5757 \times 10^{-5} T^{-0.5} - 3.4541 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	213	99	99	COMPILED
		213	267	7- 9-76

MULLITE (3-2)

FORMULA WEIGHT 426.056

3Al<sub>2</sub>O<sub>3</sub>·2SiO<sub>2</sub>: Crystals 298.15 to melting point 2133 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	269.57	269.57	326.10	38.079 *	27.974 *	-4.901
UNCERTAINTY		4.18	4.18		1.470	1.490	
400	92.275	375.60	283.32	392.41	37.839 *	24.547 *	-3.206
500	156.542	467.72	311.18	431.95	37.416 *	21.271 *	-2.222
600	204.813	549.00	344.19	458.85	36.849 *	18.104 *	-1.576
700	242.569	621.27	378.70	478.36	36.051 *	15.031 *	-1.122
800	273.006	686.15	413.14	493.13	34.909 *	12.110 *	-0.791
900	298.133	744.93	446.80	504.61	33.509 *	9.353 *	-0.543
1000	319.249	798.58	479.33	513.73	33.589 *	6.669 *	-0.348
1100	337.275	847.90	510.63	521.06	33.686 *	3.951 *	-0.188
1200	352.847	893.50	540.65	527.02	33.726 *	1.277 *	-0.056
1300	366.438	935.89	569.45	531.88	33.661 *	-1.438 *	0.058
1400	378.400	975.45	597.05	535.85	33.449 *	-4.127 *	0.154
1500	389.011	1012.54	623.53	539.09	33.037 *	-6.833 *	0.238
1600	398.476	1047.42	648.94	541.73	32.415 *	-9.439 *	0.308
1700	406.968	1080.33	673.36	543.85	31.546 *	-12.022 *	0.369
1800	414.621	1111.46	696.84	545.53	30.411 *	-14.555 *	0.422

MELTING POINT	2133	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	13.4550 J/bar 134.550 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 7.5455 \times 10^2 - 2.9426 \times 10^{-2} T - 6.5757 \times 10^3 T^{-0.5} - 3.4541 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	213	99	99	COMPILED
		213	267	7- 9-76



LARNITE

FORMULA WEIGHT 172.244

Ca<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to 970 K. α crystals (bredigite) 970 to 1710 K.

α crystals 1710 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>p</sub> <sup>o</sup> J/mol·K			
298.15	0.000	127.61	127.61	128.60	-2305.980	-2191.264	383.902
UNCERTAINTY		0.84	0.84		3.220	3.225	0.565
400	35.025	167.91	132.89	145.21	-2305.414	-2152.126	281.040
500	58.216	201.56	143.34	156.16	-2304.116	-2113.956	220.844
600	75.240	230.77	155.53	164.18	-2302.520	-2076.056	180.737
700	88.406	256.57	168.16	170.38	-2300.900	-2038.456	152.112
800	98.975	279.65	180.67	175.35	-2300.892	-2000.884	130.645
900	107.700	300.55	192.85	179.45	-2299.472	-1963.450	113.956
970	112.967	314.08	201.12	181.92	-2298.787	-1937.335	104.326
970	113.040	314.16	201.12	179.28	-2298.716	-1937.335	104.326
1000	115.048	319.64	204.59	180.66	-2298.667	-1926.167	100.613
1100	121.354	337.21	215.86	185.28	-2298.502	-1888.940	89.699
1200	126.837	353.50	226.66	189.89	-2312.899	-1850.445	80.548
1300	131.663	368.67	237.01	194.50	-2309.705	-1812.053	72.809
1400	135.950	382.87	246.92	199.11	-2306.393	-1773.904	66.185
1500	139.791	396.23	256.44	203.72	-2302.973	-1735.986	60.453
1600	143.257	408.83	265.57	208.33	-2299.460	-1698.307	55.444
1700	146.406	420.76	274.35	212.94	-2346.370	-1660.403	51.018
1710	146.700	421.95	275.25	213.40	-2345.989	-1656.577	50.603
1710	159.076	434.33	275.25	205.02	-2324.826	-1656.577	50.603
1800	160.596	444.84	284.24	205.02	-2629.040	-1616.022	46.896

MELTING POINT	2403	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>		kJ	MOLAR VOLUME	5.1600 J/bar 51.600 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^o = 2.4871 \times 10^{-2} - 8.3145 \times 10^{-4} T - 2.0521 \times 10^{-3} T^{-0.5} - 9.0774 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 970 K)

$$C_p^o = 134.557 + 0.046108 T$$

(EQUATION VALID FROM 970 - 1710 K)

REFERENCE 45 120 126 COMPILED 7- 9-76

LARNITE FORMULA WEIGHT 172.244  
 =====  
 Ca<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to 970 K. α' crystals (brögigite) 970 to 1710 K.  
 α crystals 1710 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	127.61	127.61	128.60	-125.102 *	-128.002 *	22.425
UNCERTAINTY		0.84	0.84		0.960	0.970	
400	35.025	167.91	132.89	145.21	-125.222 *	-128.974 *	16.842
500	58.216	201.56	143.34	156.16	-125.366 *	-129.901 *	13.571
600	75.240	230.77	155.53	164.18	-125.485 *	-130.789 *	11.386
700	88.406	256.57	168.16	170.38	-125.625 *	-131.673 *	9.826
800	98.975	279.65	180.67	175.35	-125.836 *	-132.516 *	8.652
900	107.700	300.55	192.85	179.45	-126.072 *	-133.326 *	7.738
970	112.967	314.08	201.12	181.92	-125.769 *	-133.903 *	7.211
970	113.040	314.16	201.12	179.28	-125.698 *	-133.903 *	7.211
1000	115.048	319.64	204.59	180.66	-125.491 *	-134.171 *	7.008
1100	121.354	337.21	215.86	185.28	-124.800 *	-135.064 *	6.414
1200	126.837	353.50	226.66	189.89	-124.046 *	-136.033 *	5.921
1300	131.663	368.67	237.01	194.50	-123.254 *	-137.059 *	5.507
1400	135.950	382.87	246.92	199.11	-122.442 *	-138.165 *	5.155
1500	139.791	396.23	256.44	203.72	-121.650 *	-139.321 *	4.852
1600	143.257	408.83	265.57	208.33	-120.873 *	-140.504 *	4.587
1700	146.406	420.76	274.35	212.94	-120.133 *	-141.774 *	4.356
1710	146.700	421.95	275.25	213.40	-119.615 *	-141.901 *	4.335
1710	159.076	434.33	275.25	205.02	-98.452 *	-141.901 *	4.335
1800	160.596	444.84	284.24	205.02	-99.076 *	-145.660 *	4.227

MELTING POINT	2403	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>		kJ	MOLAR VOLUME	5.1600 J/bar 51.600 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.4871 \times 10^{-2} - 8.3145 \times 10^{-4} T - 2.0521 \times 10^{-6} T^{-0.5} - 9.0774 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 970 K)

$$C_P^0 = 134.557 + 0.046108 T$$

(EQUATION VALID FROM 970 - 1710 K)

REFERENCE	45	120	126	COMPILED 7- 9-76
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CALCIUM OLIVINE

FORMULA WEIGHT 172.244

Ca<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to 1120 K. Calcium olivine is the stable form of dicalcium silicate below 1120 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	120.50	120.50	126.80	-2316.62 <sup>o</sup>	-2199.784	385.395
UNCERTAINTY		0.84	0.84		3.920	3.950	0.692
400	34.350	160.05	125.70	141.67	-2316.324	-2159.892	282.054
500	56.820	192.74	135.92	151.21	-2315.454	-2120.884	221.568
600	73.202	220.99	147.79	158.78	-2314.383	-2082.051	181.259
700	85.911	245.98	160.07	165.44	-2313.286	-2043.429	152.483
800	96.241	268.48	172.24	171.60	-2313.719	-2004.775	130.899
900	104.944	289.03	184.09	177.48	-2312.592	-1966.202	114.116
1000	112.483	308.03	195.55	183.18	-2311.872	-1927.762	100.696
1100	119.165	325.75	206.59	188.76	-2311.550	-1889.382	89.720
1200	125.194	342.41	217.22	194.26	-2325.511	-1849.749	80.518

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	kJ	MOLAR VOLUME	5.9110 J/bar 59.110 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.3257 \times 10^{-2} + 5.2510 \times 10^{-5} T - 1.9049 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	45	120	93	COMPILED
			229	7- 9-76

## CALCIUM OLIVINE

FORMULA WEIGHT 172.244

Ca<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to 1120 K. Calcium olivine is the stable form of dicalcium silicate below 1120 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	120.50	120.50	126.80	-135.742 *	-136.522 *	23.918
UNCERTAINTY		0.84	0.84		1.000	1.020	
400	34.350	160.05	125.70	141.67	-136.132 *	-136.740 *	17.856
500	56.820	192.74	135.92	151.21	-136.704 *	-136.829 *	14.294
600	73.202	220.99	147.79	158.78	-137.348 *	-136.784 *	11.908
700	85.911	245.98	160.07	165.44	-138.011 *	-136.646 *	10.197
800	96.241	268.48	172.24	171.60	-138.663 *	-136.407 *	8.906
900	104.944	289.03	184.09	177.48	-139.192 *	-136.078 *	7.898
1000	112.483	308.03	195.55	183.18	-138.696 *	-135.766 *	7.092
1100	119.165	325.75	206.59	188.76	-137.848 *	-135.506 *	6.435
1200	125.194	342.41	217.22	194.26	-136.658 *	-135.337 *	5.891

## MELTING POINT

K

## BOILING POINT

K

## ENTHALPY OF MELTING

kJ

## ENTHALPY OF VAPORIZATION

kJ

 $H_{298}^0 - H_0^0$ 

kJ

## MOLAR VOLUME

5.9110 J/bar  
59.110 cm<sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 1.3257 \times 10^2 + 5.2510 \times 10^{-2} T - 1.9049 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1200 K)

## REFERENCE

45

120

93  
229COMPILED  
7- 9-76

GEHLENITE

FORMULA WEIGHT 274.206

Ca<sub>2</sub>Al<sub>2</sub>SiO<sub>7</sub>: Crystals 298.15 to melting point 1863 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	209.80	209.80	206.40	-4007.570	-3808.705	667.272
UNCERTAINTY		1.64	1.64		2.820	2.900	0.508
400	56.750	275.09	218.34	236.74	-4007.948	-3740.651	488.481
500	94.752	330.07	235.32	255.46	-4006.908	-3673.938	383.815
600	122.688	377.87	255.18	268.58	-4005.317	-3607.478	314.060
700	144.259	420.04	275.78	278.35	-4003.661	-3541.319	264.258
800	161.514	457.72	296.21	285.96	-4003.721	-3475.182	226.907
900	175.689	491.77	316.08	292.06	-4002.587	-3409.174	197.864
1000	187.586	522.80	335.21	297.06	-4023.652	-3341.722	174.554
1100	197.733	551.32	353.59	301.23	-4023.617	-3273.549	155.449
1200	206.508	577.68	371.17	304.75	-4038.103	-3204.088	139.471
1300	214.183	602.20	388.02	307.76	-4034.968	-3134.719	125.955
1400	220.964	625.10	404.14	310.35	-4031.696	-3065.614	114.380
1500	226.997	646.59	419.59	312.59	-4028.312	-2996.714	104.355
1600	232.409	666.83	434.42	314.55	-4024.833	-2928.071	95.592
1700	237.292	685.95	448.66	316.26	-4071.779	-2859.212	87.853
1800	241.722	704.07	462.35	317.76	-4374.866	-2781.240	80.710

MELTING POINT	1863	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	9.0240 J/bar 90.240 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 4.0573 \times 10^{-2} - 7.0986 \times 10^{-3} T - 3.1744 \times 10^{-5} T^2 + 1.1883 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	206	273	93	COMPILED
		268	11	7- 9-76

## GEHLENITE

FORMULA WEIGHT 274.206

Ca<sub>2</sub>Al<sub>2</sub>SiO<sub>7</sub>: Crystals 298.15 to melting point 1863 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	209.80	209.80	206.40	-150.992 *	-163.215 *	28.595
UNCERTAINTY		1.64	1.64		3.090	3.170	
400	56.750	275.09	218.34	236.74	-151.452 *	-167.336 *	21.852
500	94.752	330.07	235.32	255.46	-152.174 *	-171.229 *	17.888
600	122.688	377.87	255.18	268.58	-153.018 *	-174.954 *	15.231
700	144.259	420.04	275.78	278.35	-153.982 *	-178.545 *	13.323
800	161.514	457.72	296.21	285.96	-155.100 *	-181.971 *	11.882
900	175.689	491.77	316.08	292.06	-156.322 *	-185.257 *	10.752
1000	187.586	522.80	335.21	297.06	-156.778 *	-188.438 *	9.843
1100	197.733	551.32	353.59	301.23	-157.196 *	-191.594 *	9.098
1200	206.508	577.68	371.17	304.75	-157.615 *	-194.682 *	8.474
1300	214.183	602.20	388.02	307.76	-158.060 *	-197.761 *	7.946
1400	220.964	625.10	404.14	310.35	-158.542 *	-200.809 *	7.492
1500	226.997	646.59	419.59	312.59	-159.117 *	-203.818 *	7.098
1600	232.409	666.83	434.42	314.55	-159.765 *	-206.756 *	6.750
1700	237.292	685.95	448.66	316.26	-160.513 *	-209.676 *	6.443
1800	241.722	704.07	462.35	317.76	-161.373 *	-212.547 *	6.168

MELTING POINT	1863	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	9.0240 J/bar 90.240 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 4.0573 \times 10^{-2} - 7.0986 \times 10^{-3} T - 3.1744 \times 10^{-3} T^{-0.5} - 1.1883 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	206	273	93	COMPILED
		268	11	7- 9-76

GROSSULAR

FORMULA WEIGHT 450.455

Ca<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>: Crystals 298.15 to 1200 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	255.50	255.50	330.10	-6643.140	-6281.359	1100.472
UNCERTAINTY		0.51	0.51		6.000	6.100	1.069
400	92.225	361.51	269.28	389.55	-6643.817	-6157.534	804.095
500	155.598	452.65	297.05	425.66	-6641.469	-6036.219	630.602
600	202.645	532.42	329.78	448.31	-6637.887	-5915.468	514.989
700	238.877	602.72	363.84	463.18	-6634.129	-5795.383	432.458
800	267.621	665.31	397.69	473.91	-6632.988	-5675.525	370.576
900	291.056	721.66	430.60	482.89	-6630.058	-5555.984	322.462
1000	310.680	773.00	462.32	491.71	-6649.649	-5435.229	283.909
1100	327.577	820.32	492.74	501.53	-6648.281	-5313.882	252.336
1200	342.547	864.44	521.89	513.15	-6668.283	-5190.716	225.947

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	47.047 kJ	MOLAR VOLUME	12.5300 J/bar 125.300 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.5293 \times 10^3 - 0.69900 T + 2.5300 \times 10^{-4} T^2 - 1.8943 \times 10^{-6} T^{-0.5} + 7.4426 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	152	283	286	COMPILED
			88	03-15-79

GROSSULAR

FORMULA WEIGHT 450.455

Ca<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>: Crystals 298.15 to 1200 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	255.50	255.50	330.10	-330.073 *	-319.806 *	56.029
UNCERTAINTY							
		0.51	0.51		7.320	7.560	
400	92.225	361.51	269.28	389.55	-330.953 *	-316.153 *	41.285
500	155.598	452.65	297.05	425.66	-331.550 *	-312.390 *	32.635
600	202.645	532.42	329.78	448.31	-332.225 *	-308.483 *	26.856
700	238.877	602.72	363.84	463.18	-333.384 *	-304.453 *	22.719
800	267.621	665.31	397.69	473.91	-335.272 *	-300.199 *	19.601
900	291.056	721.66	430.60	482.89	-337.703 *	-295.647 *	17.159
1000	310.680	773.00	462.32	491.71	-337.934 *	-290.974 *	15.199
1100	327.577	820.32	492.74	501.53	-337.911 *	-286.279 *	13.594
1200	342.547	864.44	521.89	513.15	-337.463 *	-281.579 *	12.257

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	47.047 kJ	MOLAR VOLUME	12.5300 J/bar 125.300 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.5293 \times 10^3 - 0.69900 T + 2.5300 \times 10^{-4} T^2 - 1.8943 \times 10^{-6} T^{-0.5} \\ + 7.4426 \times 10^{-6} T^{-2} \\ \text{(EQUATION VALID FROM 298 - 1200 K)}$$

REFERENCE	152	283	286 88	COMPILED 03-15-79
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HERWINITE

FORMULA WEIGHT 328.712

Ca<sub>2</sub>Hg(SiO<sub>4</sub>)<sub>2</sub>: Crystals 298.15 to incongruent melting point 1848 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	253.13	253.13	252.30	-4566.790	-4339.403	760.249
UNCERTAINTY		2.09	2.09		5.310	5.397	0.946
400	69.050	332.56	263.51	286.70	-4566.036	-4261.765	556.532
500	114.736	398.87	284.13	306.81	-4563.869	-4185.954	437.306
600	147.915	456.05	308.14	319.97	-4561.297	-4110.588	357.860
700	173.193	506.11	332.92	329.27	-4558.887	-4035.686	301.148
800	193.167	550.56	357.39	336.43	-4559.142	-3960.814	258.616
900	209.433	590.54	381.11	342.46	-4557.514	-3886.081	225.543
1000	223.012	626.91	403.90	348.02	-4565.941	-3810.761	199.055
1100	234.625	660.34	425.71	353.53	-4566.383	-3735.257	177.373
1200	244.773	691.35	446.58	359.31	-4588.577	-3657.764	159.219
1300	253.822	720.35	466.53	365.59	-4584.197	-3580.404	143.863
1400	262.050	747.70	485.65	372.52	-4706.302	-3499.798	130.580
1500	269.667	773.66	503.99	380.24	-4699.695	-3413.832	118.881
1600	276.842	798.47	521.63	388.85	-4692.423	-3328.342	108.660

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	10.4400 J/bar 104.400 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

MAGNESIUM.. M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 6.5076 \times 10^{-2} - 0.18169 T + 7.0357 \times 10^{-5} T^2 - 6.0529 \times 10^{-8} T^{-0.5}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	206	273	179	COMPILED
			116	7- 9-76

## HERWINITE

FORMULA WEIGHT 328.712

Ca<sub>2</sub>Hg(SiO<sub>4</sub>)<sub>2</sub>: Crystals 298.15 to incongruent melting point 1848 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	253.13	253.13	252.30	-238.633 *	-247.170 *	43.303
UNCERTAINTY		2.09	2.09		1.590	1.600	
400	69.050	332.56	263.51	286.70	-238.823 *	-250.059 *	32.654
500	114.736	398.87	284.13	306.81	-239.172 *	-252.837 *	26.414
600	147.915	456.05	308.14	319.97	-239.765 *	-255.514 *	22.245
700	173.193	506.11	332.92	329.27	-240.736 *	-258.075 *	19.258
800	193.167	550.56	357.39	336.43	-242.174 *	-260.461 *	17.006
900	209.433	590.54	381.11	342.46	-243.933 *	-262.618 *	15.242
1000	223.012	626.91	403.90	348.02	-244.234 *	-264.684 *	13.826
1100	234.625	660.34	425.71	353.53	-244.413 *	-266.723 *	12.666
1200	244.773	691.35	446.58	359.31	-244.447 *	-268.746 *	11.698
1300	253.822	720.35	466.53	365.59	-244.277 *	-270.769 *	10.880
1400	262.050	747.70	485.65	372.52	-243.813 *	-272.852 *	10.180
1500	269.667	773.66	503.99	380.24	-243.003 *	-274.954 *	9.575
1600	276.842	798.47	521.63	388.85	-241.717 *	-277.092 *	9.046

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	10.4400 J/bar 104.400 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 6.5076 \times 10^{-2} - 0.18169 T + 7.0357 \times 10^{-5} T^2 - 6.0529 \times 10^{-8} T^{-0.5}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	206	273	179	COMPILED
			116	7- 9-76

AKERNAMITE

FORMULA WEIGHT 272.633

Ca<sub>2</sub>HgSi<sub>2</sub>O<sub>7</sub>: Crystals 298.15 to melting point 1727 K.

TEMP. K	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>P</sub> <sup>o</sup> J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	209.33	209.33	212.00	-3876.520	-3679.069	644.560
UNCERTAINTY		2.09	2.09		2.830	2.850	0.499
400	57.600	275.62	218.02	238.34	-3876.213	-3611.616	471.631
500	95.540	330.73	235.19	255.18	-3874.839	-3545.624	370.410
600	123.200	378.38	255.18	267.22	-3873.058	-3479.928	302.956
700	144.457	420.29	275.83	276.41	-3871.239	-3414.566	254.799
800	161.427	457.69	296.26	283.80	-3871.063	-3349.260	218.685
900	175.378	491.49	316.11	290.04	-3869.523	-3284.102	190.605
1000	187.125	522.34	335.21	295.54	-3877.575	-3218.355	168.110
1100	197.212	550.75	353.54	300.56	-3877.235	-3152.478	149.699
1200	206.023	577.10	371.08	305.31	-3891.343	-3085.312	134.301
1300	213.839	601.72	387.88	309.93	-3887.717	-3018.318	121.278
1400	220.864	624.86	404.00	314.51	-4010.766	-2948.014	109.992
1500	227.263	646.72	419.46	319.14	-4005.352	-2872.279	100.022
1600	233.152	667.46	434.31	323.88	-3999.609	-2796.913	91.310
1700	238.633	687.24	448.61	328.78	-4094.524	-2721.052	83.608

MELTING POINT	1727	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>		kJ	MOLAR VOLUME	9.2810 J/bar 92.810 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

MAGNESIUM.. M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^o = 4.4511x10^2 - 5.1463x10^{-2} T + 2.1857x10^{-5} T^2 - 3.7937x10^3 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1700 K)

REFERENCE	206	273	178	COMPILED
			116	7- 9-76

## AKERMANITE

FORMULA WEIGHT 272.633

Ca<sub>2</sub>MgSi<sub>2</sub>O<sub>7</sub>: Crystals 298.15 to melting point 1727 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	209.33	209.33	212.00	-183.452 *	-190.323 *	33.344
UNCERTAINTY		2.09	2.09		0.920	0.930	
400	57.600	275.62	218.02	238.34	-183.672 *	-192.656 *	25.158
500	95.540	330.73	235.19	255.18	-184.247 *	-194.837 *	20.355
600	123.200	378.38	255.18	267.22	-185.095 *	-196.879 *	17.140
700	144.457	420.29	275.83	276.41	-186.250 *	-198.759 *	14.832
800	161.427	457.69	296.26	283.80	-187.768 *	-200.448 *	13.088
900	175.378	491.49	316.11	290.04	-189.512 *	-201.915 *	11.719
1000	187.125	522.34	335.21	295.54	-189.705 *	-203.285 *	10.619
1100	197.212	550.75	353.54	300.56	-189.750 *	-204.646 *	9.718
1200	206.023	577.10	371.08	305.31	-189.671 *	-205.991 *	8.967
1300	213.839	601.72	387.88	309.93	-189.469 *	-207.356 *	8.332
1400	220.864	624.86	404.00	314.51	-189.132 *	-208.762 *	7.789
1500	227.263	646.72	419.46	319.14	-188.661 *	-210.187 *	7.319
1600	233.152	667.46	434.31	323.88	-188.021 *	-211.605 *	6.908
1700	238.633	687.24	448.61	328.78	-187.192 *	-213.117 *	6.548

MELTING POINT	1727	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	9.2810 J/bar 92.810 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 4.4511 \times 10^2 - 5.1463 \times 10^{-2} T + 2.1857 \times 10^{-5} T^2 - 3.7937 \times 10^3 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1700 K)

REFERENCE	206	273	178	COMPILED
			116	7- 9-76

TITANITE (SPHENE)

FORMULA WEIGHT 196.063

CaTiSiO<sub>6</sub>: Crystals 298.15 to melting point 1670 K. Liquid 1670 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	129.20	129.20	139.00	-2601.400	-2459.855	430.958
UNCERTAINTY		0.84	0.84		2.380	2.430	0.426
400	38.600	173.59	134.99	161.33	-2600.913	-2411.527	314.915
500	64.382	210.92	146.54	172.69	-2599.490	-2364.345	247.002
600	83.077	243.09	160.01	179.96	-2597.787	-2317.464	201.754
700	97.313	271.25	173.94	185.28	-2596.079	-2270.888	169.456
800	108.585	296.28	187.69	189.58	-2595.225	-2224.454	145.243
900	117.789	318.82	201.03	193.27	-2593.723	-2178.177	126.419
1000	125.510	339.36	213.85	196.59	-2592.562	-2132.072	111.368
1100	132.114	358.24	226.13	199.67	-2591.763	-2086.071	99.060
1200	137.865	375.74	237.88	202.58	-2602.320	-2039.336	88.770
1300	142.952	392.07	249.12	205.38	-2599.572	-1992.551	80.062
1400	147.507	407.39	259.88	208.09	-2596.764	-1945.975	72.606
1500	151.635	421.84	270.21	210.73	-2593.886	-1899.580	66.150
1600	155.410	435.52	280.11	213.33	-2590.938	-1853.394	60.507
1670	157.779	444.98	287.20	215.13	-2589.005	-1821.898	56.986
1670	231.914	519.11	287.20	279.50	-2465.200	-1821.898	56.986
1700	232.754	523.89	291.14	279.50	-2512.860	-1809.510	55.600
1800	235.350	539.82	304.47	279.50	-2656.740	-1764.949	51.218

MELTING POINT	1670	K	BOILING POINT	K
ENTHALPY OF MELTING	123.805	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>		kJ	MOLAR VOLUME	5.5650 J/bar 55.650 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

TITANIUM... ALPHA-BETA 1155, M. P. 1943 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.7673 \times 10^2 + 2.3852 \times 10^{-2} T - 3.9905 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1670 K)

REFERENCE	132	120	93 253	COMPILED 7- 9-76
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## TITANITE (SPHENE)

FORMULA WEIGHT 196.063

CaTiSiO<sub>6</sub>: Crystals 298.15 to melting point 1670 K. Liquid 1670 to 1800 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	129.20	129.20	139.00	-110.861 *	-110.634 *	19.383
UNCERTAINTY		0.84	0.84		1.520	1.540	
400	38.600	173.59	134.99	161.33	-110.951 *	-110.531 *	14.434
500	64.382	210.92	146.54	172.69	-110.951 *	-110.431 *	11.537
600	83.077	243.09	160.01	179.96	-111.052 *	-110.314 *	9.604
700	97.313	271.25	173.94	185.28	-111.343 *	-110.181 *	8.222
800	108.585	296.28	187.69	189.58	-111.863 *	-109.983 *	7.181
900	117.789	318.82	201.03	193.27	-112.551 *	-109.698 *	6.367
1000	125.510	339.36	213.85	196.59	-112.493 *	-109.383 *	5.714
1100	132.114	358.24	226.13	199.67	-112.414 *	-109.071 *	5.179
1200	137.865	375.74	237.88	202.58	-112.322 *	-108.771 *	4.735
1300	142.952	392.07	249.12	205.38	-112.221 *	-108.477 *	4.359
1400	147.507	407.39	259.88	208.09	-112.111 *	-108.206 *	4.037
1500	151.635	421.84	270.21	210.73	-112.014 *	-107.935 *	3.759
1600	155.410	435.52	280.11	213.33	-111.913 *	-107.640 *	3.514
1670	157.779	444.98	287.20	215.13	-111.955 *	-107.993 *	3.378
1670	231.914	519.11	287.20	279.50	11.850 *	-107.993 *	3.378
1700	232.754	523.89	291.14	279.50	13.746 *	-109.945 *	3.378
1800	235.350	539.82	304.47	279.50	20.067 *	-117.327 *	3.405

MELTING POINT	1670 K	BOILING POINT	K
ENTHALPY OF MELTING	123.805 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	5.5650 J/bar 55.650 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE OXIDES			

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.7673 \times 10^2 + 2.3852 \times 10^{-2} T - 3.9905 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1670 K)

REFERENCE	132	120	93	COMPILED
			253	7- 9-76

FAYALITE

FORMULA WEIGHT 203.778

Fe<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to melting point 1490 K. Liquid 1490 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	148.32	148.32	132.90	-1479.360	-1379.375	241.662
UNCERTAINTY		1.67	1.67		2.410	2.470	0.432
400	36.625	190.46	153.83	152.30	-1478.226	-1345.361	175.687
500	60.836	225.60	164.76	162.14	-1476.520	-1312.315	137.097
600	78.293	255.77	177.48	168.70	-1474.794	-1279.627	111.402
700	91.593	282.18	190.59	173.95	-1473.253	-1247.269	93.073
800	102.186	305.72	203.53	178.71	-1472.103	-1215.071	79.336
900	110.944	327.04	216.10	183.37	-1471.590	-1182.918	68.655
1000	118.426	346.60	228.17	188.14	-1472.267	-1150.821	60.113
1100	124.988	364.76	239.77	193.13	-1474.434	-1118.527	53.115
1200	130.885	381.79	250.90	198.42	-1474.452	-1086.235	47.283
1300	136.295	397.90	261.61	204.06	-1471.098	-1054.104	42.355
1400	141.350	413.24	271.89	210.07	-1467.417	-1022.201	38.139
1490	145.163	425.70	280.53	215.81	-1464.465	-993.164	34.817
1490	207.024	487.56	280.53	240.60	-1372.292	-993.164	34.817
1500	207.247	489.11	281.86	240.60	-1371.630	-990.572	34.495
1600	209.331	504.63	295.30	240.60	-1365.007	-965.401	31.517
1700	211.169	519.23	308.06	240.60	-1411.469	-940.134	28.887
1800	212.803	533.00	320.20	240.60	-1405.691	-912.531	26.481

MELTING POINT	1490	K	BOILING POINT	K
ENTHALPY OF MELTING	92.173	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>		kJ	MOLAR VOLUME	4.6390 J/bar 46.390 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

IRON..... CURIE P. 1042, ALPHA-GAMMA 1184, GAMMA-DELTA 1665,  
M. P. DELTA 1809 K.  
SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.7276 \times 10^2 - 3.4055 \times 10^{-3} T + 2.2411 \times 10^{-6} T^2 - 3.6299 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1490 K)

REFERENCE	190	251	93	COMPILED
		120	127	8-27-76

## FAYALITE

FORMULA WEIGHT 203.778

Fe<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to melting point 1490 K. Liquid 1490 to 1800 K.

TEMP.	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	148.32	148.32	132.90	-24.574 *	-20.775 *	3.640
UNCERTAINTY		1.67	1.67				
400	36.625	190.46	153.83	152.30	-25.314 *	-19.358 *	2.528
500	60.836	225.60	164.76	162.14	-25.718 *	-17.809 *	1.860
600	78.293	255.77	177.48	168.70	-26.199 *	-16.185 *	1.409
700	91.593	282.18	190.59	173.95	-26.850 *	-14.469 *	1.080
800	102.186	305.72	203.53	178.71	-27.687 *	-12.641 *	0.825
900	110.944	327.04	216.10	183.37	-28.604 *	-10.697 *	0.621
1000	118.426	346.60	228.17	188.14	-28.651 *	-8.715 *	0.455
1100	124.988	364.76	239.77	193.13	-28.496 *	-6.716 *	0.319
1200	130.885	381.79	250.90	198.42	-28.099 *	-4.760 *	0.207
1300	136.295	397.90	261.61	204.06	-27.415 *	-2.820 *	0.113
1400	141.350	413.24	271.89	210.07	-26.394 *	-0.974 *	0.036
1490	145.163	425.70	280.53	215.81	-25.911 *	1.084 *	-0.038
1490	207.024	487.56	280.53	240.60	66.262 *	1.084 *	-0.038
1500	207.247	489.11	281.86	240.60	66.651 *	0.697 *	-0.024
1600	209.331	504.63	295.30	240.60	70.540 *	-3.824 *	0.125
1700	211.169	519.23	308.06	240.60	29.468 *	-3.124 *	0.096
1800	212.803	533.00	320.20	240.60	32.238 *	-5.188 *	0.151

MELTING POINT	1490	K	BOILING POINT		K
ENTHALPY OF MELTING	92.173	kJ	ENTHALPY OF VAPORIZATION		kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	4.6390	J/bar cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

FeO..... H. P. 1650 K.

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.7276 \times 10^2 - 3.4055 \times 10^{-3} T + 2.2411 \times 10^{-5} T^2 - 3.6299 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1490 K)

REFERENCE	190	251	93	COMPILED
		120	127	8-27-76



FORSTERITE

FORMULA WEIGHT 140.694

Mg<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to melting point 2163 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	95.19	95.19	117.90	-2170.370	-2051.325	359.385
UNCERTAINTY		0.84	0.84		1.325	1.345	0.236
400	32.600	132.68	100.08	136.53	-2170.730	-2010.566	262.554
500	54.618	164.47	109.85	148.09	-2170.223	-1970.578	205.866
600	70.915	192.24	121.33	156.32	-2169.281	-1930.726	168.085
700	83.583	216.83	133.25	162.61	-2168.114	-1891.067	141.114
800	93.785	238.88	145.10	167.63	-2166.838	-1851.575	120.896
900	102.233	258.87	156.64	171.80	-2165.522	-1812.218	105.179
1000	109.365	277.16	167.79	175.33	-2182.126	-1771.526	92.535
1100	115.505	294.01	178.51	178.39	-2180.644	-1730.534	82.177
1200	120.859	309.65	188.79	181.09	-2178.997	-1689.674	73.550
1300	125.587	324.25	198.66	183.50	-2177.196	-1648.995	66.258
1400	129.800	337.93	208.13	185.68	-2429.185	-1601.239	59.743
1500	133.594	350.80	217.21	187.66	-2424.752	-1542.240	53.706
1600	137.031	362.97	225.94	189.48	-2420.205	-1483.534	48.433
1700	140.165	374.51	234.34	191.16	-2466.061	-1424.709	43.776
1800	143.042	385.48	242.44	192.73	-2461.018	-1363.610	39.571

MELTING POINT	2163	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	17.276	kJ	MOLAR VOLUME	4.3790 J/bar 43.790 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.2798 \times 10^2 + 3.4139 \times 10^{-3} T - 1.7446 \times 10^3 T^{-0.5} - 8.9397 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	190	120	93	COMPILED
			128	7-13-76

## FORSTERITE

FORMULA WEIGHT 140.694

Mg<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to melting point 2163 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>p</sub> <sup>0</sup> J/mol·K			
298.15	0.000	95.19	95.19	117.90	-56.690 *	-56.645 *	9.924
UNCERTAINTY		0.84	0.84		0.610	0.660	
400	32.600	132.68	100.08	136.53	-56.880 *	-56.612 *	7.393
500	54.618	164.47	109.85	148.09	-57.079 *	-56.509 *	5.903
600	70.915	192.24	121.33	156.32	-57.322 *	-56.380 *	4.908
700	83.583	216.83	133.25	162.61	-57.637 *	-56.194 *	4.193
800	93.785	238.88	145.10	167.63	-58.070 *	-55.974 *	3.655
900	102.233	258.87	156.64	171.80	-58.560 *	-55.663 *	3.231
1000	109.365	277.16	167.79	175.33	-58.240 *	-55.360 *	2.892
1100	115.505	294.01	178.51	178.39	-57.810 *	-55.094 *	2.616
1200	120.859	309.65	188.79	181.09	-57.296 *	-54.873 *	2.389
1300	125.587	324.25	198.66	183.50	-56.709 *	-54.706 *	2.198
1400	129.800	337.93	208.13	185.68	-56.060 *	-54.563 *	2.036
1500	133.594	350.80	217.21	187.66	-55.337 *	-54.482 *	1.897
1600	137.031	362.97	225.94	189.48	-54.554 *	-54.443 *	1.777
1700	140.165	374.51	234.34	191.16	-53.704 *	-54.452 *	1.673
1800	143.042	385.48	242.44	192.73	-52.783 *	-54.546 *	1.583

MELTING POINT	2163	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	17.276	kJ	MOLAR VOLUME	4.3790 J/bar 43.790 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 2.2798 \times 10^2 + 3.4139 \times 10^{-3} T - 1.7446 \times 10^3 T^{-0.5} - 8.9397 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	190	120	93	COMPILED
			128	7-13-76

PYROPE

FORMULA WEIGHT 403.130

Mg<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>: Crystals 298.15 to 1200 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	260.76	260.76	325.50	-6284.620	-5932.412	1039.341
UNCERTAINTY		10.00	10.00		6.000	7.000	1.226
400	91.250	365.63	274.38	385.20	-6285.621	-5811.810	758.948
500	153.722	455.57	301.85	419.38	-6283.764	-5693.564	594.806
600	199.935	534.09	334.16	441.07	-6280.657	-5575.782	485.417
700	235.469	603.22	367.75	455.29	-6277.167	-5458.593	407.327
800	263.571	664.67	401.10	464.62	-6273.814	-5341.880	348.791
900	286.267	719.77	433.50	470.55	-6270.958	-5225.529	303.284
1000	304.885	769.54	464.66	473.99	-6317.003	-5105.693	266.696
1100	320.341	814.80	494.46	475.54	-6314.698	-4984.686	236.704
1200	333.287	856.19	522.90	475.63	-6312.676	-4863.835	211.719

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
$H_{298}^0 - H_0^0$	KJ	MOLAR VOLUME	11.3270 J/bar 113.270 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM... M. P. 922, B. P. 1361 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 8.0258 \times 10^{-2} - 9.5795 \times 10^{-2} T - 7.2873 \times 10^{-3} T^{-0.5} - 2.3522 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	252	285	31	COMPILED
		252		03-15-79

## PYROPE

FORMULA WEIGHT 403.130

Mg<sub>3</sub>Al<sub>2</sub>Si<sub>2</sub>O<sub>12</sub>: Crystals 298.15 to 1200 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	260.76	260.76	325.50	-72.350 *	-73.732 *	12.918
UNCERTAINTY		10.00	10.00		4.950	5.950	
400	91.250	365.63	274.38	385.20	-72.270 *	-74.226 *	9.693
500	153.722	455.57	301.85	419.38	-72.254 *	-74.714 *	7.806
600	199.935	534.09	334.16	441.07	-72.609 *	-75.177 *	6.545
700	235.469	603.22	367.75	455.29	-73.619 *	-75.529 *	5.635
800	263.571	664.67	401.10	464.62	-75.530 *	-75.706 *	4.942
900	286.267	719.77	433.50	470.55	-78.260 *	-75.543 *	4.385
1000	304.885	769.54	464.66	473.99	-79.223 *	-75.183 *	3.928
1100	320.341	814.80	494.46	475.54	-80.630 *	-74.737 *	3.548
1200	333.287	856.19	522.90	475.63	-82.584 *	-74.114 *	3.227

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	11.3270 J/bar 113.270 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 8.0258 \times 10^{-2} - 9.5795 \times 10^{-2} T - 7.2873 \times 10^{-5} T^{-0.5} - 2.3522 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	252	285	31	COMPILED
		252		03-15-79

CORDIERITE

FORMULA WEIGHT 584.957

Mg<sub>2</sub>Al<sub>2</sub>(AlSi<sub>4</sub>O<sub>14</sub>): Crystals 298.15 to 1700 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T	S <sub>T</sub> <sup>o</sup>	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T	C <sub>P</sub> <sup>o</sup>	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	407.20	407.20	452.30	-9161.524	-8651.112	1515.645
UNCERTAINTY		3.80	3.80		5.850	5.900	1.034
400	127.125	553.31	426.18	537.34	-9164.054	-8476.171	1106.879
500	214.440	678.89	464.45	586.54	-9162.518	-8304.353	867.554
600	279.428	788.99	509.56	620.40	-9159.031	-8133.000	708.044
700	330.036	886.62	556.58	645.93	-9154.564	-7962.358	594.161
800	370.842	974.25	603.41	666.39	-9149.651	-7792.357	508.791
900	404.656	1053.76	649.10	683.53	-9144.646	-7622.957	442.427
1000	433.303	1126.56	693.26	698.34	-9200.284	-7449.584	389.128
1100	458.005	1193.74	735.74	711.46	-9193.912	-7274.828	345.454
1200	479.627	1256.16	776.53	723.30	-9186.852	-7100.620	309.083
1300	498.793	1314.49	815.70	734.14	-9179.137	-6927.084	278.335
1400	515.964	1369.27	853.31	744.19	-9424.739	-6747.032	251.736
1500	531.497	1420.94	889.44	753.59	-9413.451	-6556.126	228.306
1600	545.658	1469.86	924.20	762.47	-9401.602	-6366.013	207.830
1700	558.662	1516.34	957.68	770.90	-9641.738	-6174.551	189.722

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	kJ	MOLAR VOLUME	23.3220 J/bar 233.220 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

- MAGNESIUM.. M. P. 922, B. P. 1361 K.
- ALUMINUM... M. P. 933 K.
- SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^o = 8.2134 \times 10^2 + 4.3339 \times 10^{-2} T - 5.0003 \times 10^{-5} T^2 - 8.2112 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1700 K)

REFERENCE 206 273 31 COMPILED 7-13-76

## CORDIERITE

FORMULA WEIGHT 584.957

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 $\text{Mg}_2\text{Al}_3(\text{AlSi}_5\text{O}_{18})$ : Crystals 298.15 to 1700 K.  
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TEMP.	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	407.20	407.20	452.30	-53.644 *	-66.824 *	11.707
UNCERTAINTY		3.80	3.80		1.450	1.470	
400	127.125	553.31	426.18	537.34	-54.204 *	-71.252 *	9.305
500	214.440	678.89	464.45	586.54	-55.246 *	-75.396 *	7.877
600	279.428	788.99	509.56	620.40	-56.956 *	-79.265 *	6.901
700	330.036	886.62	556.58	645.93	-59.470 *	-82.800 *	6.179
800	370.842	974.25	603.41	666.39	-62.908 *	-85.924 *	5.610
900	404.656	1053.76	649.10	683.53	-66.914 *	-88.525 *	5.138
1000	433.303	1126.56	693.26	698.34	-66.994 *	-90.914 *	4.749
1100	458.005	1193.74	735.74	711.46	-66.712 *	-93.336 *	4.432
1200	479.627	1256.16	776.53	723.30	-66.133 *	-95.764 *	4.169
1300	498.793	1314.49	815.70	734.14	-65.303 *	-98.270 *	3.949
1400	515.964	1369.27	853.31	744.19	-64.244 *	-100.828 *	3.762
1500	531.497	1420.94	889.44	753.59	-63.008 *	-103.523 *	3.605
1600	545.658	1469.86	924.20	762.47	-61.580 *	-106.220 *	3.468
1700	558.662	1516.34	957.68	770.90	-59.986 *	-109.063 *	3.351

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	23.3220 J/bar 233.220 $\text{cm}^3$

## TRANSITIONS IN REFERENCE STATE OXIDES

$\text{SiO}_2$ ..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 8.2134 \times 10^{-2} + 4.3339 \times 10^{-2} T - 5.0003 \times 10^{-3} T^{0.5} - 8.2112 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1700 K)

REFERENCE	206	273	31	COMPILED 7-13-76
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TEPHROITE

FORMULA WEIGHT 201.960

Mn<sub>2</sub>SiO<sub>4</sub>: Crystals 298.15 to melting point 1620 K. Liquid 1620 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>p</sub> <sup>o</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	163.20	163.20	129.87	-1728.070	-1629.695	285.517
UNCERTAINTY		4.20	4.20		3.180	3.430	0.601
400	34.975	203.46	168.49	144.50	-1727.838	-1596.114	208.432
500	58.052	236.96	178.91	155.61	-1727.064	-1563.264	163.314
600	74.993	266.06	191.07	163.31	-1726.026	-1530.600	133.251
700	88.007	291.65	203.64	168.53	-1724.943	-1498.114	111.791
800	98.307	314.40	216.09	172.07	-1723.952	-1465.777	95.706
900	106.644	334.82	228.18	174.57	-1723.120	-1433.545	83.201
1000	113.540	353.32	239.78	176.46	-1726.913	-1401.333	73.198
1100	119.335	370.21	250.88	178.10	-1726.447	-1368.803	64.999
1200	124.298	385.78	261.48	179.71	-1726.022	-1336.288	58.167
1300	128.628	400.23	271.60	181.50	-1725.618	-1303.834	52.389
1400	132.479	413.76	281.28	183.61	-1729.759	-1271.288	47.433
1500	135.969	426.51	290.54	186.15	-1734.194	-1238.278	43.121
1600	139.197	438.62	299.42	189.21	-1758.908	-1203.882	39.303
1620	139.783	441.54	301.76	189.89	-1759.059	-1197.982	38.627
1620	195.131	496.89	301.76	243.10	-1669.395	-1197.982	38.627
1700	197.388	508.00	310.61	243.10	-1715.998	-1173.273	36.050
1800	199.928	521.89	321.96	243.10	-1710.890	-1141.476	33.125

MELTING POINT	1620 K	BOILING POINT	K
ENTHALPY OF MELTING	89.663 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	kJ	MOLAR VOLUME	4.8610 J/bar 48.610 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.  
SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^o = 5.1252 \times 10^{-2} - 0.18273 T + 5.2058 \times 10^{-5} T^2 - 6.6404 \times 10^{-8} T^{-0.5} + 4.6026 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1620 K)

REFERENCE	160	120	93	COMPILED
			111	7-15-76

## TEPHROITE

FORMULA WEIGHT 201.960

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 $\text{Mn}_2\text{SiO}_4$ : Crystals 298.15 to melting point 1620 K. Liquid 1620 to 1800 K.  
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TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY	FREE ENERGY	Log $K_f$
					kJ/mol	kJ/mol	
298.15	0.000	163.20	163.20	129.87	-46.930 *	-47.615 *	8.342
UNCERTAINTY		4.20	4.20		2.000	2.020	
400	34.975	203.46	168.49	144.50	-47.250 *	-47.806 *	6.243
500	58.052	236.96	178.91	155.61	-47.448 *	-47.913 *	5.005
600	74.993	266.06	191.07	163.31	-47.593 *	-47.995 *	4.178
700	88.007	291.65	203.64	168.53	-47.844 *	-48.054 *	3.586
800	98.307	314.40	216.09	172.07	-48.330 *	-48.042 *	3.137
900	106.644	334.82	228.18	174.57	-49.050 *	-47.979 *	2.785
1000	113.540	353.32	239.78	176.46	-49.129 *	-47.849 *	2.499
1100	119.335	370.21	250.88	178.10	-49.301 *	-47.706 *	2.265
1200	124.298	385.78	261.48	179.71	-49.563 *	-47.560 *	2.070
1300	128.628	400.23	271.60	181.50	-49.897 *	-47.375 *	1.904
1400	132.479	413.76	281.28	183.61	-50.270 *	-47.163 *	1.760
1500	135.969	426.51	290.54	186.15	-50.641 *	-46.920 *	1.634
1600	139.197	438.62	299.42	189.21	-50.951 *	-46.662 *	1.523
1620	139.783	441.54	301.76	189.89	-50.907 *	-47.211 *	1.522
1620	195.131	496.89	301.76	243.10	38.756 *	-47.211 *	1.522
1700	197.388	508.00	310.61	243.10	42.601 *	-50.916 *	1.564
1800	199.928	521.89	321.96	243.10	47.407 *	-56.544 *	1.641

MELTING POINT	1620 K	BOILING POINT	K
ENTHALPY OF MELTING	89.663 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	4.8610 J/bar 48.610 $\text{cm}^3$

## TRANSITIONS IN REFERENCE STATE OXIDES

$\text{SiO}_2$ ..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 5.1252 \times 10^{-2} - 0.18273 T + 5.2058 \times 10^{-5} T^2 - 6.6404 \times 10^{-8} T^{-0.5} \\ + 4.6026 \times 10^{-6} T^{-2} \\ \text{(EQUATION VALID FROM 298 - 1620 K)}$$

REFERENCE	160	120	93	COMPILED
			111	7-15-76



ZIRCON FORMULA WEIGHT 183.304

ZrSiO<sub>4</sub>: Tetragonal crystals 298.15 to 1800 K. Note zircon decomposes to ZrO<sub>2</sub> and SiO<sub>2</sub> at approximately 1949 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>p</sub> <sup>o</sup> J/mol·K			
298.15	0.000	84.03	84.03	98.60	-2033.400	-1918.890	336.183
UNCERTAINTY		1.25	1.25		1.000	1.040	0.182
400	27.425	115.57	88.14	115.47	-2033.329	-1879.753	245.472
500	46.166	142.55	96.38	125.99	-2032.420	-1841.455	192.376
600	60.108	166.20	106.09	133.22	-2031.051	-1803.381	156.999
700	70.943	187.15	116.21	138.41	-2029.422	-1765.564	131.749
800	79.627	205.89	126.26	142.23	-2027.655	-1727.984	112.826
900	86.744	222.81	136.07	145.08	-2025.839	-1690.626	98.122
1000	92.694	238.22	145.53	147.21	-2024.019	-1653.489	86.370
1100	97.725	252.32	154.59	148.78	-2022.250	-1616.515	76.762
1200	102.030	265.32	163.29	149.93	-2024.290	-1579.475	68.753
1300	105.747	277.36	171.61	150.72	-2022.298	-1542.507	61.979
1400	108.979	288.55	179.57	151.23	-2020.335	-1505.696	56.178
1500	111.807	298.99	187.18	151.51	-2018.413	-1468.977	51.155
1600	114.292	308.77	194.48	151.59	-2016.549	-1432.421	46.764

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	14.903 kJ	MOLAR VOLUME	3.9260 J/bar 39.260 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

ZIRCONIUM.. ALPHA-BETA 1136, M. P. 2125 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^o = 2.3695 \times 10^2 - 1.7879 \times 10^{-2} T - 2.2678 \times 10^3 T^{-0.5} - 1.4960 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	115	120	264	COMPILED
			234	7-13-76

## ZIRCON

FORMULA WEIGHT 183.304

ZrSiO<sub>4</sub>: Tetragonal crystals 298.15 to 1800 K. Note zircon decomposes to  
ZrO<sub>2</sub> and SiO<sub>2</sub> at approximately 1949 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	84.03	84.03	98.60	-22.140 *	-19.812 *	3.471
UNCERTAINTY		1.25	1.25		2.010	2.050	
400	27.425	115.57	88.14	115.47	-22.340 *	-18.980 *	2.479
500	46.166	142.55	96.38	125.99	-22.482 *	-18.127 *	1.894
600	60.108	166.20	106.09	133.22	-22.629 *	-17.241 *	1.501
700	70.943	187.15	116.21	138.41	-22.864 *	-16.333 *	1.219
800	79.627	205.89	126.26	142.23	-23.257 *	-15.369 *	1.004
900	86.744	222.81	136.07	145.08	-23.780 *	-14.348 *	0.833
1000	92.694	238.22	145.53	147.21	-23.559 *	-13.319 *	0.696
1100	97.725	252.32	154.59	148.78	-23.342 *	-12.288 *	0.584
1200	102.030	265.32	163.29	149.93	-23.165 *	-11.298 *	0.492
1300	105.747	277.36	171.61	150.72	-23.053 *	-10.326 *	0.415
1400	108.979	288.55	179.57	151.23	-23.030 *	-9.352 *	0.349
1500	111.807	298.99	187.18	151.51	-28.977 *	-8.330 *	0.290
1600	114.292	308.77	194.48	151.59	-28.715 *	-6.943 *	0.227

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	14.903 kJ	MOLAR VOLUME	3.9260 J/bar 39.260 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

ZrO<sub>2</sub>..... MONOCLINIC TO TETRAGONAL CRYSTAL 1478 K.SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.3695 \times 10^2 - 1.7879 \times 10^{-2} T - 2.2678 \times 10^3 T^{-0.5} - 1.4960 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	115	120	264 234	COMPILED 7-13-76
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WOLLASTONITE

FORMULA WEIGHT 116.164

CaSiO<sub>3</sub>: Crystals 298.15 to 1400 K. Pseudowollastonite is the stable phase above 1398 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	82.01	82.01	85.27	-1635.220	-1549.903	271.538
UNCERTAINTY		0.84	0.84		1.435	1.455	0.255
400	23.900	109.49	85.59	100.48	-1634.971	-1520.765	198.592
500	40.052	132.81	92.76	108.08	-1634.080	-1492.315	155.902
600	51.813	152.96	101.15	112.85	-1633.018	-1464.049	127.457
700	60.789	170.63	109.84	116.28	-1631.979	-1435.980	107.155
800	67.902	186.34	118.44	119.01	-1631.789	-1407.954	91.930
900	73.711	200.50	126.79	121.32	-1630.931	-1380.021	80.095
1000	78.578	213.39	134.81	123.38	-1630.394	-1352.174	70.631
1100	82.738	225.24	142.50	125.28	-1630.186	-1324.375	62.890
1200	86.358	236.21	149.85	127.06	-1637.250	-1295.929	56.411
1300	89.555	246.45	156.89	128.76	-1635.498	-1267.573	50.932
1400	92.414	256.06	163.65	130.41	-1633.657	-1239.362	46.241

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.9930 J/bar 39.930 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, H. P. BETA 1112, B. P. 1755 K.

SILICON.... H. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.1125 \times 10^{-2} + 1.4373 \times 10^{-5} T + 16.936 T^{-0.5} - 2.7779 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	240	120	254 19	COMPILED 7-13-76
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## WOLLASTONITE

FORMULA WEIGHT 116.164

CaSiO<sub>3</sub>: Crystals 298.15 to 1400 K. Pseudowollastonite is the stable phase above 1398 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	82.01	82.01	85.27	-89.431 *	-90.128 *	15.790
UNCERTAINTY		0.84	0.84		0.540	0.860	
400	23.900	109.49	85.59	100.48	-89.451 *	-90.359 *	11.800
500	40.052	132.81	92.76	108.08	-89.435 *	-90.590 *	9.464
600	51.813	152.96	101.15	112.85	-89.552 *	-90.806 *	7.905
700	60.789	170.63	109.84	116.28	-89.866 *	-91.000 *	6.791
800	67.902	186.34	118.44	119.01	-90.406 *	-91.126 *	5.950
900	73.711	200.50	126.79	121.32	-91.101 *	-91.173 *	5.292
1000	78.578	213.39	134.81	123.38	-91.055 *	-91.185 *	4.763
1100	82.738	225.24	142.50	125.28	-90.969 *	-91.201 *	4.331
1200	86.358	236.21	149.85	127.06	-90.855 *	-91.215 *	3.970
1300	89.555	246.45	156.89	128.76	-90.719 *	-91.252 *	3.667
1400	92.414	256.06	163.65	130.41	-90.561 *	-91.318 *	3.407

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	3.9930 J/bar 39.930 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.1125 \times 10^2 + 1.4373 \times 10^{-2} T + 16.936 T^{-0.5} - 2.7779 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	240	120	254	COMPILED
			19	7-13-76

PSEUDONOLLASTONITE

FORMULA WEIGHT 116.164

CaSiO<sub>3</sub>: Crystals 298.15 to melting point 1817 K.

TEMP. K	FORMATION FROM THE ELEMENTS				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	87.45	87.45	86.48	-1628.650	-1544.955	270.671
UNCERTAINTY		0.84	0.84		2.594	2.636	0.462
400	23.925	114.96	91.03	99.74	-1628.391	-1516.373	198.019
500	39.834	138.03	98.20	106.65	-1627.619	-1488.464	155.499
600	51.372	157.90	106.53	111.21	-1626.713	-1460.708	127.166
700	60.176	175.31	115.13	114.65	-1625.838	-1433.115	106.941
800	67.167	190.81	123.64	117.50	-1625.807	-1405.548	91.773
900	72.900	204.80	131.90	120.00	-1625.091	-1378.051	79.980
1000	77.728	217.56	139.83	122.28	-1624.674	-1350.624	70.550
1100	81.877	229.32	147.44	124.43	-1624.563	-1323.240	62.836
1200	85.509	240.23	154.72	126.48	-1631.699	-1295.202	56.379
1300	88.738	250.44	161.70	128.47	-1629.991	-1267.253	50.919
1400	91.643	260.03	168.39	130.40	-1628.167	-1239.430	46.244
1500	94.293	269.09	174.80	132.30	-1626.211	-1211.715	42.196
1600	96.727	277.69	180.96	134.17	-1624.132	-1184.156	38.659
1700	98.985	285.88	186.90	136.02	-1672.430	-1156.285	35.528

MELTING POINT	1817	K	BOILING POINT	K
ENTHALPY OF MELTING	27.405	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	4.0080 J/bar 40.080 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 1.0710 \times 10^2 + 1.7481 \times 10^{-2} T - 2.2965 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1700 K)

REFERENCE	115	120	116	COMPILED 8-27-76
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## PSEUDOWOLLASTONITE

FORMULA WEIGHT 116.164

CaSiO<sub>3</sub>: Crystals 298.15 to melting point 1817 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	87.45	87.45	86.48	-82.861 *	-85.180 *	14.923
UNCERTAINTY		0.84	0.84				
400	23.925	114.96	91.03	99.74	-82.871 *	-85.967 *	11.226
500	39.834	138.03	98.20	106.65	-82.974 *	-86.739 *	9.062
600	51.372	157.90	106.53	111.21	-83.247 *	-87.465 *	7.615
700	60.176	175.31	115.13	114.65	-83.725 *	-88.135 *	6.577
800	67.167	190.81	123.64	117.50	-84.424 *	-88.720 *	5.793
900	72.900	204.80	131.90	120.00	-85.261 *	-89.203 *	5.177
1000	77.728	217.56	139.83	122.28	-85.335 *	-89.635 *	4.682
1100	81.877	229.32	147.44	124.43	-85.346 *	-90.066 *	4.277
1200	85.509	240.23	154.72	126.48	-85.304 *	-90.488 *	3.939
1300	88.738	250.44	161.70	128.47	-85.212 *	-90.932 *	3.654
1400	91.643	260.03	168.39	130.40	-85.071 *	-91.386 *	3.410
1500	94.293	269.09	174.80	132.30	-84.889 *	-91.834 *	3.198
1600	96.727	277.69	180.96	134.17	-84.663 *	-92.295 *	3.013
1700	98.985	285.88	186.90	136.02	-84.395 *	-92.793 *	2.851

MELTING POINT	1817	K	BOILING POINT	K
ENTHALPY OF MELTING	27.405	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	4.0080 J/bar 40.080 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.0710 \times 10^2 + 1.7481 \times 10^{-2} T - 2.2965 \times 10^{-6} T^2$$

(EQUATION VALID FROM 298 - 1700 K)

REFERENCE	115	120	116	COMPILED 8-27-76
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Ca-Al PYROXENE

FORMULA WEIGHT 218.126

CaAl<sub>2</sub>SiO<sub>6</sub>: Crystals 298.15 to 1700 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	156.00	156.00	157.03	-3275.680	-3103.770	543.770
UNCERTAINTY							
		4.00	4.00		2.761	2.971	0.521
400	45.575	208.32	162.74	195.65	-3276.395	-3044.840	397.617
500	77.626	254.18	176.55	214.21	-3275.223	-2987.078	312.059
600	101.380	294.28	192.90	225.29	-3273.414	-2929.602	255.045
700	119.650	329.61	209.96	232.84	-3271.505	-2872.463	214.347
800	134.166	361.09	226.92	238.50	-3270.509	-2815.485	183.833
900	146.022	389.45	243.43	243.07	-3269.026	-2758.683	160.111
1000	155.925	415.27	259.35	246.97	-3289.440	-2700.510	141.061
1100	164.360	438.97	274.61	250.41	-3288.404	-2641.670	125.443
1200	171.664	460.89	289.23	253.56	-3294.562	-2582.280	112.404
1300	178.078	481.31	303.23	256.49	-3291.829	-2523.035	101.377
1400	183.779	500.42	316.64	259.27	-3288.940	-2464.033	91.934
1500	188.900	518.40	329.50	261.93	-3285.888	-2405.206	83.757
1600	193.545	535.38	341.83	264.51	-3282.679	-2346.597	76.608

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	6.3500 J/bar 63.500 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.3240 \times 10^2 + 2.1845 \times 10^{-2} T - 7.2788 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	285	88	286	88	COMPILED
					03-15-79

## Ca-Al PYROXENE

FORMULA WEIGHT 218.126

CaAl<sub>2</sub>SiO<sub>6</sub>: Crystals 298.15 to 1700 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	156.00	156.00	157.03	-54.191 *	-61.767 *	10.821
UNCERTAINTY		4.00	4.00		2.040	2.080	
400	45.575	208.32	162.74	195.65	-54.571 *	-64.271 *	8.393
500	77.626	254.18	176.55	214.21	-54.594 *	-66.699 *	6.968
600	101.380	294.28	192.90	225.29	-54.684 *	-69.102 *	6.016
700	119.650	329.61	209.96	232.84	-54.987 *	-71.493 *	5.335
800	134.166	361.09	226.92	238.50	-55.560 *	-73.816 *	4.820
900	146.022	389.45	243.43	243.07	-56.331 *	-76.041 *	4.414
1000	155.925	415.27	259.35	246.97	-56.403 *	-78.233 *	4.087
1100	164.360	438.97	274.61	250.41	-56.468 *	-80.416 *	3.818
1200	171.664	460.89	289.23	253.56	-56.532 *	-82.572 *	3.594
1300	178.078	481.31	303.23	256.49	-56.592 *	-84.749 *	3.405
1400	183.779	500.42	316.64	259.27	-56.641 *	-86.924 *	3.243
1500	188.900	518.40	329.50	261.93	-56.694 *	-89.094 *	3.103
1600	193.545	535.38	341.83	264.51	-56.728 *	-91.223 *	2.978

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	6.3500 J/bar 63.500 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.3240 \times 10^2 + 2.1845 \times 10^{-2} T - 7.2788 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	285	88	286	88	COMPILED	03-15-79
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DIOPSIDE

FORMULA WEIGHT 216.553

CaMg(SiO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to melting point 1664 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	143.09	143.09	166.52	-3210.760	-3036.554	531.994
UNCERTAINTY		0.84	0.84		9.120	9.160	1.605
400	46.400	196.45	150.05	194.83	-3210.800	-2976.984	388.756
500	77.808	241.77	163.96	210.81	-3209.587	-2918.662	304.912
600	100.950	281.24	180.29	221.96	-3207.850	-2860.617	249.040
700	118.877	316.13	197.25	230.60	-3205.893	-2802.910	209.157
800	133.300	347.40	214.10	237.70	-3204.605	-2745.390	179.256
900	145.244	375.76	230.52	243.72	-3202.512	-2688.092	156.013
1000	155.356	401.71	246.35	248.90	-3209.601	-2630.281	137.392
1100	164.069	425.65	261.58	253.39	-3207.899	-2572.451	122.156
1200	171.678	447.87	276.19	257.27	-3213.333	-2514.107	109.437
1300	178.394	468.59	290.20	260.59	-3209.850	-2455.994	98.683
1400	184.364	488.01	303.65	263.38	-3333.180	-2394.565	89.343
1500	189.714	506.26	316.55	265.67	-3328.236	-2327.674	81.057
1600	194.521	523.47	328.95	267.48	-3323.214	-2261.133	73.819

MELTING POINT	1664.50 K	BOILING POINT	K
ENTHALPY OF MELTING	77.404 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	6.6090 J/bar 66.090 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

MAGNESIUM.. M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.9182 \times 10^2 + 8.3079 \times 10^{-2} T - 2.1718 \times 10^{-5} T^2 - 4.2795 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	115	120	148 178	COMPILED 10-29-76
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## DIOPSID

FORMULA WEIGHT 216.553

CaMg(SiO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to melting point 1664 K.

TEMP. K	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	143.09	143.09	166.52	-152.781 *	-151.295 *	26.506
UNCERTAINTY		0.84	0.84		8.850	8.900	
400	46.400	196.45	150.05	194.83	-152.931 *	-150.771 *	19.689
500	77.808	241.77	163.96	210.81	-153.100 *	-150.205 *	15.692
600	100.950	281.24	180.29	221.96	-153.456 *	-149.592 *	13.023
700	118.877	316.13	197.25	230.60	-154.065 *	-148.906 *	11.112
800	133.300	347.40	214.10	237.70	-154.982 *	-148.118 *	9.671
900	145.244	375.76	230.52	243.72	-156.071 *	-147.180 *	8.542
1000	155.356	401.71	246.35	248.90	-155.568 *	-146.218 *	7.638
1100	164.069	425.65	261.58	253.39	-154.899 *	-145.320 *	6.901
1200	171.678	447.87	276.19	257.27	-154.119 *	-144.484 *	6.289
1300	178.394	468.59	290.20	260.59	-153.273 *	-143.705 *	5.774
1400	184.364	488.01	303.65	263.38	-152.401 *	-143.009 *	5.336
1500	189.714	506.26	316.55	265.67	-151.546 *	-142.366 *	4.958
1600	194.521	523.47	328.95	267.48	-150.743 *	-141.767 *	4.628

MELTING POINT	1664.50 K	BOILING POINT	K
ENTHALPY OF MELTING	77.404 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	6.6090 J/bar 66.090 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.9182 \times 10^2 + 8.3079 \times 10^{-2} T - 2.1718 \times 10^{-5} T^2 - 4.2795 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	115	120	148	COMPILED
			178	10-29-76

$\alpha$ -SPODUMENE

FORMULA WEIGHT 186.090

$\text{LiAlSi}_2\text{O}_6$ : Crystals 298.15 to 1200 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	129.30	129.30	158.90	-3053.500	-2880.203	504.602
UNCERTAINTY		0.80	0.80		2.790	2.800	0.490
400	43.925	179.80	135.88	184.70	-3054.521	-2820.797	368.360
500	74.022	223.11	149.09	203.21	-3057.381	-2762.071	288.553
600	96.763	261.45	164.69	217.09	-3056.322	-2703.090	235.326
700	114.746	295.75	181.00	227.74	-3054.560	-2644.353	197.325
800	129.414	326.72	197.31	236.09	-3052.332	-2585.884	168.842
900	141.644	354.93	213.29	242.72	-3049.822	-2527.725	146.706
1000	152.032	380.79	228.76	248.04	-3057.801	-2469.101	128.973
1100	160.963	404.64	243.68	252.34	-3054.684	-2410.380	114.460
1200	168.727	426.75	258.02	255.82	-3051.373	-2351.930	102.377

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.8370 J/bar 58.370 $\text{cm}^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

LITHIUM.... H. P. 453.69, B. P. 1618 K.

ALUMINUM... H. P. 933 K.

SILICON.... H. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 4.2117 \times 10^2 - 2.4005 \times 10^{-2} T - 4.7761 \times 10^3 T^{-0.5} + 1.9100 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	211	211	93	COMPILED
			15	9-13-76

$\alpha$ -SPODUMENE

FORMULA WEIGHT 186.090

LiAlSi<sub>2</sub>O<sub>6</sub>: Crystals 298.15 to 1200 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	129.30	129.30	158.90	-94.885 *	-95.520 *	16.735
UNCERTAINTY		0.80	0.80		2.300	2.315	
400	43.925	179.80	135.88	184.70	-94.885 *	-95.749 *	12.504
500	74.022	223.11	149.09	203.21	-95.152 *	-95.942 *	10.023
600	96.763	261.45	164.69	217.09	-95.562 *	-96.061 *	8.363
700	114.746	295.75	181.00	227.74	-96.181 *	-96.101 *	7.171
800	129.414	326.72	197.31	236.09	-97.103 *	-96.027 *	6.270
900	141.644	354.93	213.29	242.72	-98.240 *	-95.815 *	5.561
1000	152.032	380.79	228.76	248.04	-97.843 *	-95.568 *	4.992
1100	160.963	404.64	243.68	252.34	-97.386 *	-95.363 *	4.528
1200	168.727	426.75	258.02	255.82	-96.933 *	-95.200 *	4.144

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.8370 J/bar 58.370 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 4.2117 \times 10^{-2} - 2.4005 \times 10^{-2} T - 4.7761 \times 10^3 T^{-0.5} + 1.9100 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	211	211	93	COMPILED
			15	9-13-76

$\beta$ -SPODUMENE

FORMULA WEIGHT 186.090

$\text{LiAlSi}_2\text{O}_6$ : Crystals 298.15 to 1700 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	154.40	154.40	162.80	-3025.300	-2859.487	500.972
UNCERTAINTY		1.20	1.20		2.790	2.805	0.490
400	45.125	206.28	161.15	189.61	-3025.841	-2802.709	365.998
500	75.894	250.61	174.72	207.37	-3028.245	-2746.685	286.945
600	98.942	289.62	190.68	220.38	-3026.815	-2690.485	234.229
700	117.036	324.38	207.34	230.42	-3024.757	-2634.591	196.596
800	131.726	355.69	223.96	238.43	-3022.282	-2579.010	168.393
900	143.956	384.17	240.21	245.01	-3019.542	-2523.761	146.476
1000	154.347	410.27	255.92	250.51	-3027.286	-2468.066	128.919
1100	163.308	434.37	271.06	255.20	-3023.904	-2412.303	114.551
1200	171.137	456.76	285.62	259.24	-3020.281	-2356.850	102.591
1300	178.053	477.65	299.60	262.76	-3016.449	-2301.722	92.485
1400	184.214	497.24	313.03	265.86	-3012.443	-2246.925	83.834
1500	189.753	515.68	325.93	268.60	-3008.271	-2192.374	76.346
1600	194.759	533.09	338.33	271.05	-3003.964	-2138.121	69.803
1700	199.312	549.59	350.28	273.25	-3245.573	-2076.045	63.789

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	7.8250 J/bar 78.250 $\text{cm}^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

LITHIUM.... M. P. 453.69, B. P. 1618 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 3.6281 \times 10^2 - 3.6841 \times 10^{-3} T - 3.4346 \times 10^3 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1700 K)

REFERENCE	211	211	93	COMPILED
			15	9- 8-76

$\beta$ -SPODUMENE

FORMULA WEIGHT 186.090

LiAlSi<sub>2</sub>O<sub>6</sub>: Crystals 298.15 to 1700 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	154.40	154.40	162.80	-66.685 *	-74.804 *	13.105
UNCERTAINTY		1.20	1.20		2.300	2.320	
400	45.125	206.28	161.15	189.61	-66.205 *	-77.661 *	10.141
500	75.894	250.61	174.72	207.37	-66.016 *	-80.556 *	8.416
600	98.942	289.62	190.68	220.38	-66.055 *	-83.456 *	7.265
700	117.036	324.38	207.34	230.42	-66.378 *	-86.339 *	6.443
800	131.726	355.69	223.96	238.43	-67.053 *	-89.153 *	5.821
900	143.956	384.17	240.21	245.01	-67.960 *	-91.851 *	5.331
1000	154.347	410.27	255.92	250.51	-67.328 *	-94.533 *	4.938
1100	163.308	434.37	271.06	255.20	-66.606 *	-97.286 *	4.620
1200	171.137	456.76	285.62	259.24	-65.841 *	-100.120 *	4.358
1300	178.053	477.65	299.60	262.76	-65.068 *	-103.002 *	4.139
1400	184.214	497.24	313.03	265.86	-64.315 *	-105.951 *	3.953
1500	189.753	515.68	325.93	268.60	-63.616 *	-108.953 *	3.794
1600	194.759	533.09	338.33	271.05	-62.981 *	-111.973 *	3.656
1700	199.312	549.59	350.28	273.25	-62.435 *	-115.066 *	3.536

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	7.8250 J/bar 78.250 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 3.6281 \times 10^2 - 3.6841 \times 10^{-3} T - 3.4346 \times 10^3 T^{-0.5}$$

(EQUATION VALID FROM 298 - 1700 K)

REFERENCE	211	211	93	COMPILED
			15	9- 8-76

EUCRYPTITE

FORMULA WEIGHT 126.006

LiAlSiO<sub>4</sub>: α-eucryptite 298.15 to 1300 K. β-eucryptite 1300 to 1600 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	103.80	103.80	113.30	-2123.300	-2009.174	352.000
UNCERTAINTY		0.80	0.80		1.980	1.990	0.348
400	32.025	140.59	108.57	136.03	-2123.903	-1970.047	257.263
500	54.286	172.52	118.23	149.79	-2126.521	-1931.316	201.764
600	71.047	200.73	129.68	159.38	-2125.464	-1892.364	164.746
700	84.201	225.86	141.66	166.56	-2123.922	-1853.631	138.320
800	94.864	248.48	153.62	172.20	-2122.081	-1815.129	118.516
900	103.722	269.04	165.32	176.79	-2120.072	-1776.876	103.128
1000	111.224	287.87	176.65	180.61	-2128.640	-1738.100	90.789
1100	117.684	305.24	187.56	183.86	-2126.146	-1699.158	80.687
1200	123.319	321.36	198.04	186.67	-2123.467	-1660.448	72.278
1300	128.642	336.34	207.70	191.20	-2120.170	-1621.438	65.150
1400	133.543	350.89	217.35	200.83	-2116.492	-1583.135	59.068
1500	138.295	365.01	226.72	208.75	-2112.137	-1545.166	53.808
1600	142.946	378.74	235.79	216.67	-2107.066	-1507.544	49.216

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.3630 J/bar 53.630 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

LITHIUM... M. P. 453.69, B. P. 1618 K.

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATIONS

$$C_p^0 = 2.4697 \times 10^2 - 2.0577 \times 10^3 T^{-0.5} - 1.2895 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1300 K)

$$C_p^0 = 89.943 + 7.9203 \times 10^{-2} T$$

(EQUATION VALID FROM 1300 - 1600 K)

REFERENCE	211	211	93	COMPILED
			15	9- 8-76

## EUCRYPTITE

FORMULA WEIGHT 126.006

LiAlSiO<sub>4</sub>: α Eucryptite 298.15 to 1300 K. Eucryptite 1300 to 1600 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	103.80	103.80	113.30	-75.385 *	-80.779 *	14.152
UNCERTAINTY		0.80	0.80		2.105	2.115	
400	32.025	140.59	108.57	136.03	-75.115 *	-82.659 *	10.794
500	54.286	172.52	118.23	149.79	-74.832 *	-84.582 *	8.836
600	71.047	200.73	129.68	159.38	-74.601 *	-86.554 *	7.535
700	84.201	225.86	141.66	166.56	-74.495 *	-88.555 *	6.608
800	94.864	248.48	153.62	172.20	-74.563 *	-90.559 *	5.913
900	103.722	269.04	165.32	176.79	-74.750 *	-92.539 *	5.371
1000	111.224	287.87	176.65	180.61	-74.184 *	-94.549 *	4.939
1100	117.684	305.24	187.56	183.86	-73.580 *	-96.615 *	4.588
1200	123.319	321.36	198.04	186.67	-72.964 *	-98.734 *	4.298
1300	128.642	336.34	207.70	191.20	-71.897 *	-100.367 *	4.033
1400	133.543	350.89	217.35	200.83	-70.605 *	-102.511 *	3.825
1500	138.295	365.01	226.72	208.75	-68.803 *	-104.840 *	3.651
1600	142.946	378.74	235.79	216.67	-66.435 *	-107.315 *	3.503

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.3630 J/bar 53.630 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 2.4697 \times 10^2 - 2.0577 \times 10^3 T^{-0.5} - 1.2895 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1300 K)

$$C_P^0 = 89.943 + 7.9203 \times 10^{-2} T$$

(EQUATION VALID FROM 1300 - 1600 K)

REFERENCE	211	211	93	COMPILED
			15	9- 8-76



CLINOENSTATITE

FORMULA WEIGHT 100.389

MgSiO<sub>3</sub>: Crystals 298.15 to melting point 1830 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	67.86	67.86	82.09	-1547.750	-1460.883	255.942
UNCERTAINTY		0.42	0.42		1.215	1.225	0.215
400	22.350	93.58	71.23	93.01	-1548.099	-1431.137	186.888
500	37.336	115.25	77.91	101.18	-1547.927	-1401.912	146.457
600	48.517	134.27	85.75	107.39	-1547.414	-1372.745	119.509
700	57.284	151.20	93.92	112.19	-1546.686	-1343.693	100.268
800	64.391	166.44	102.05	115.95	-1545.830	-1314.755	85.845
900	70.289	180.27	109.98	118.93	-1544.911	-1285.909	74.633
1000	75.278	192.93	117.65	121.30	-1552.917	-1256.427	65.629
1100	79.551	204.58	125.03	123.19	-1551.881	-1226.831	58.258
1200	83.252	215.37	132.12	124.70	-1550.774	-1197.321	52.118
1300	86.488	225.40	138.91	125.90	-1549.616	-1167.924	46.928
1400	89.336	234.77	145.43	126.85	-1675.393	-1135.021	42.248
1500	91.865	243.54	151.68	127.57	-1673.000	-1096.489	38.183
1600	94.114	251.79	157.68	128.11	-1670.609	-1058.122	34.544

MELTING POINT	1830	K	BOILING POINT	K
ENTHALPY OF MELTING	61.505	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	12.113	kJ	MOLAR VOLUME	3.1470 J/bar 31.470 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM... M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.0556 \times 10^{-2} - 1.2796 \times 10^{-2} T - 2.2977 \times 10^{-3} T^{-0.5} + 1.1926 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	115	120	93	COMPILED
			254	8-26-76

## CLINOENSTATITE

FORMULA WEIGHT 100.389

H<sub>2</sub>SiO<sub>3</sub>: Crystals 298.15 to melting point 1830 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	67.86	67.86	82.09	-35.560 *	-35.399 *	6.202
UNCERTAINTY		0.42	0.42		0.630	0.650	
400	22.350	93.58	71.23	93.01	-35.750 *	-35.330 *	4.614
500	37.336	115.25	77.91	101.18	-36.085 *	-35.180 *	3.675
600	48.517	134.27	85.75	107.39	-36.486 *	-34.962 *	3.044
700	57.284	151.20	93.92	112.19	-36.972 *	-34.669 *	2.587
800	64.391	166.44	102.05	115.95	-37.591 *	-34.311 *	2.240
900	70.289	180.27	109.98	118.93	-38.300 *	-33.846 *	1.964
1000	75.278	192.93	117.65	121.30	-38.223 *	-33.353 *	1.742
1100	79.551	204.58	125.03	123.19	-38.098 *	-32.874 *	1.561
1200	83.252	215.37	132.12	124.70	-37.955 *	-32.412 *	1.411
1300	86.488	225.40	138.91	125.90	-37.819 *	-31.956 *	1.284
1400	89.336	234.77	145.43	126.85	-37.710 *	-31.509 *	1.176
1500	91.865	243.54	151.68	127.57	-37.632 *	-31.062 *	1.082
1600	94.114	251.79	157.68	128.11	-37.608 *	-30.616 *	1.000

MELTING POINT	1830 K	BOILING POINT	K
ENTHALPY OF MELTING	61.505 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	12.113 kJ	MOLAR VOLUME	3.1470 J/bar 31.470 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 2.0556 \times 10^2 - 1.2796 \times 10^{-2} T - 2.2977 \times 10^{-5} T^{-0.5} + 1.1926 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1600 K)

REFERENCE	115	120	93 254	COMPILED 8-26-76
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RHODONITE

FORMULA WEIGHT 131.022

MnSiO<sub>3</sub>: Crystals 298.15 to melting point 1564 K.

TEMP. K	FORMATION FROM THE ELEMENTS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>p</sub> <sup>0</sup> J/mol·K			
298.15	0.000	102.50	102.50	86.44	-1319.350	-1243.081	217.784
UNCERTAINTY		2.10	2.10		1.310	1.440	0.252
400	24.175	130.30	106.12	101.42	-1319.148	-1216.938	158.916
500	40.426	153.79	113.36	108.73	-1318.411	-1191.466	124.472
600	52.213	174.04	121.83	113.29	-1317.542	-1166.153	101.523
700	61.186	191.77	130.58	116.61	-1316.668	-1140.996	85.143
800	68.287	207.52	139.23	119.31	-1315.829	-1115.954	72.865
900	74.089	221.71	147.62	121.67	-1315.025	-1091.007	63.321
1000	78.957	234.64	155.68	123.83	-1316.469	-1066.119	55.689
1100	83.130	246.54	163.41	125.87	-1315.702	-1041.130	49.439
1200	86.773	257.58	170.81	127.83	-1314.875	-1016.190	44.234
1300	90.005	267.89	177.88	129.74	-1313.982	-991.349	39.833
1400	92.914	277.57	184.66	131.63	-1315.295	-966.500	36.061
1500	95.555	286.72	191.17	133.50	-1316.717	-941.491	32.786

MELTING POINT	1564	K	BOILING POINT	K
ENTHALPY OF MELTING		KJ	ENTHALPY OF VAPORIZATION	KJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>		KJ	MOLAR VOLUME	3.5160 J/bar 35.160 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MANGANESE.. ALPHA-BETA 980, BETA-GAMMA 1360, GAMMA-DELTA 1410,  
M. P. DELTA 1517 K.  
SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 99.043 + 1.9145 \times 10^{-2} T + 2.7447 \times 10^{-5} T^2 - 3.0407 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	115	285	93	COMPILED
	241		127	7-13-76

## RHODONITE

FORMULA WEIGHT 131.022

MnSiO<sub>3</sub>: Crystals 298.15 to melting point 1564 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS							
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	102.50	102.50	86.44	-23.430 *	-23.897 *	4.187	
UNCERTAINTY		2.10	2.10		0.710	0.960		
400	24.175	130.30	106.12	101.42	-23.430 *	-23.954 *	3.128	
500	40.426	153.79	113.36	108.73	-23.333 *	-24.093 *	2.517	
600	52.213	174.04	121.83	113.29	-23.377 *	-24.241 *	2.110	
700	61.186	191.77	130.58	116.61	-23.643 *	-24.378 *	1.819	
800	68.287	207.52	139.23	119.31	-24.163 *	-24.443 *	1.596	
900	74.089	221.71	147.62	121.67	-24.860 *	-24.437 *	1.418	
1000	78.957	234.64	155.68	123.83	-24.826 *	-24.386 *	1.274	
1100	83.130	246.54	163.41	125.87	-24.763 *	-24.345 *	1.156	
1200	86.773	257.58	170.81	127.83	-24.677 *	-24.318 *	1.059	
1300	90.005	267.89	177.88	129.74	-24.568 *	-24.295 *	0.976	
1400	92.914	277.57	184.66	131.63	-24.430 *	-24.263 *	0.905	
1500	95.555	286.72	191.17	133.50	-24.280 *	-24.264 *	0.845	

MELTING POINT	1564	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	3.5160 J/bar 35.160 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 99.043 + 1.9145 \times 10^{-2} T + 2.7447 \times 10^{-5} T^{1.5} - 3.0407 \times 10^{-8} T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	115	285	93	COMPILED
	241		127	7-13-76

JADEITE

FORMULA WEIGHT 202.140

NaAl(SiO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	133.47	133.47	159.95	-3029.400	-2850.834	499.456
UNCERTAINTY		1.25	1.25		4.180	4.230	0.741
400	44.725	184.87	140.14	188.44	-3033.114	-2789.270	364.243
500	75.266	228.87	153.60	205.34	-3032.857	-2728.337	285.029
600	97.977	267.40	169.42	217.10	-3031.734	-2667.516	232.229
700	115.656	301.56	185.90	225.98	-3030.084	-2606.934	194.533
800	129.906	332.22	202.31	233.09	-3028.105	-2546.617	166.278
900	141.711	360.02	218.31	238.99	-3025.928	-2486.541	144.316
1000	151.696	385.47	233.77	244.05	-3034.310	-2425.980	126.721
1100	160.297	408.94	248.64	248.47	-3031.621	-2365.274	112.318
1200	167.813	430.74	262.93	252.42	-3126.141	-2302.757	100.237
1300	174.461	451.09	276.63	255.99	-3122.193	-2234.316	89.776

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	6.0400 J/bar 60.400 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 3.0113 \times 10^2 + 1.0143 \times 10^{-2} T - 2.0551 \times 10^3 T^{-0.5} - 2.2393 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	115	120	97 149	COMPILED 7-13-76
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## JADEITE

FORMULA WEIGHT 202.140

NaAl(SiO<sub>3</sub>)<sub>2</sub>: Crystals 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	133.47	133.47	159.95	-162.740 *	-159.000 *	27.856
UNCERTAINTY		1.25	1.25		2.380	2.400	
400	44.725	184.87	140.14	188.44	-163.140 *	-157.660 *	20.588
500	75.266	228.87	153.60	205.34	-163.737 *	-156.232 *	16.321
600	97.977	267.40	169.42	217.10	-164.622 *	-154.644 *	13.463
700	115.656	301.56	185.90	225.98	-165.873 *	-152.891 *	11.409
800	129.906	332.22	202.31	233.09	-167.547 *	-150.935 *	9.855
900	141.711	360.02	218.31	238.99	-169.505 *	-148.716 *	8.631
1000	151.696	385.47	233.77	244.05	-169.975 *	-146.390 *	7.647
1100	160.297	408.94	248.64	248.47	---	---	---
1200	167.813	430.74	262.93	252.42	---	---	---
1300	174.461	451.09	276.63	255.99	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	6.0400 J/bar 60.400 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

Na<sub>2</sub>O..... M. P. 1193 K.SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 3.0113 \times 10^{-2} + 1.0143 \times 10^{-2} T - 2.0551 \times 10^{-5} T^2 - 2.2393 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	115	120	97	COMPILED
			149	7-13-76

TREMOLITE

FORMULA WEIGHT 812.374

Ca<sub>2</sub>Mg<sub>5</sub>[Si<sub>8</sub>O<sub>22</sub>](OH)<sub>2</sub>: Crystals 298.15 to 1100 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	548.90	548.90	655.63	-12355.080	-11627.910	2037.170
UNCERTAINTY		1.25	1.25		17.320	17.360	3.041
400	182.900	759.12	576.22	774.84	-12356.640	-11378.298	1485.860
500	309.508	940.88	631.37	850.59	-12351.782	-11134.232	1163.190
600	403.765	1100.30	696.54	895.89	-12343.991	-10891.365	948.182
700	476.370	1240.82	764.45	926.91	-12335.242	-10649.984	794.715
800	534.475	1366.46	831.98	956.04	-12327.561	-10409.676	679.685
900	583.180	1480.95	897.77	992.15	-12317.399	-10170.383	590.276
1000	626.419	1587.91	961.49	1041.50	-12350.187	-9928.687	518.624
1100	667.067	1690.18	1023.11	1108.67	-12334.212	-9687.325	460.015

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	97.646 kJ	MOLAR VOLUME	27.2920 J/bar 272.920 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

MAGNESIUM.. M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 6.1310 \times 10^3 - 4.1890 T + 1.7568 \times 10^{-3} T^2 - 8.5656 \times 10^{-6} T^3 + 5.1385 \times 10^{-9} T^4$$

(EQUATION VALID FROM 298 - 1100 K)

REFERENCE	151	228	270	COMPILED 7-13-76
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## TREMOLITE

FORMULA WEIGHT 812.374

Ca<sub>2</sub>Hg<sub>3</sub>(Si<sub>6</sub>O<sub>22</sub>(OH)<sub>2</sub>: Crystals 298.15 to 1100 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K			
298.15	0.000	548.90	548.90	655.63	-506.022 *	-487.511 *	85.410
UNCERTAINTY		1.25	1.25		15.200	15.200	
400	182.900	759.12	576.22	774.84	-550.171 *	-476.907 *	62.278
500	309.508	940.88	631.37	850.59	-548.922 *	-458.692 *	47.919
600	403.765	1100.30	696.54	895.89	-547.764 *	-440.760 *	38.372
700	476.370	1240.82	764.45	926.91	-547.856 *	-422.940 *	31.560
800	534.475	1366.46	831.98	956.04	-549.441 *	-405.040 *	26.447
900	583.180	1480.95	897.77	992.15	-551.239 *	-386.750 *	22.447
1000	626.419	1587.91	961.49	1041.50	-544.678 *	-368.798 *	19.264
1100	667.067	1690.18	1023.11	1108.67	-533.667 *	-351.733 *	16.703

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	97.646 kJ	MOLAR VOLUME	27.2920 J/bar 272.920 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.H<sub>2</sub>O..... B. P. 373.15 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 6.1310 \times 10^3 - 4.1890 T + 1.7568 \times 10^{-3} T^2 - 8.5656 \times 10^{-6} T^{\circ.5} + 5.1385 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 298 - 1100 K)

REFERENCE	151	228	270	COMPILED 7-13-76
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ANORTHITE

FORMULA WEIGHT 278.211

CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>: Crystals 298.15 to melting point 1830 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	199.30	199.30	211.40	-4229.100	-4003.326	701.369
UNCERTAINTY		0.30	0.30		3.125	3.145	0.551
400	58.975	267.10	208.12	248.31	-4229.633	-3926.038	512.691
500	99.192	325.04	225.85	270.22	-4228.388	-3850.273	402.237
600	129.013	375.71	246.70	285.18	-4226.342	-3774.824	328.629
700	152.151	420.54	268.39	296.30	-4223.993	-3699.763	276.081
800	170.746	460.71	289.96	305.21	-4222.356	-3624.941	236.686
900	186.122	497.11	310.99	312.60	-4220.036	-3550.385	206.060
1000	199.138	530.43	331.29	319.18	-4239.416	-3474.566	181.494
1100	210.399	561.21	350.81	325.49	-4237.126	-3398.199	161.368
1200	220.323	589.87	369.55	331.86	-4241.787	-3321.390	144.577
1300	229.220	616.76	387.54	338.52	-4237.278	-3244.871	130.381
1400	237.321	642.15	404.83	345.63	-4232.291	-3168.755	118.228
1500	244.810	666.27	421.46	353.34	-4226.764	-3092.956	107.707
1600	251.821	689.31	437.49	361.74	-4220.657	-3017.582	98.514
1700	258.466	711.42	452.95	370.92	-4314.917	-2941.741	90.389
1800	264.836	732.74	467.90	380.44	-4460.376	-2857.785	82.931

MELTING POINT	1830 K	BOILING POINT	K
ENTHALPY OF MELTING	81.000 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	33.333 kJ	MOLAR VOLUME	10.0790 J/bar 100.790 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 5.1683 \times 10^2 - 9.2492 \times 10^{-2} T + 4.1883 \times 10^{-5} T^2 - 4.5885 \times 10^3 T^{-0.5} - 1.4085 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	152	227	286	COMPILED
	56		93	03-15-79

## ANORTHITE

FORMULA WEIGHT 278.211

CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>: Crystals 298.15 to melting point 1830 K.

TEMP. K	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	199.30	199.30	211.40	-96.911 *	-105.035 *	18.402
UNCERTAINTY		0.30	0.30		3.430	3.450	
400	58.975	267.10	208.12	248.31	-96.961 *	-107.809 *	14.079
500	99.192	325.04	225.85	270.22	-97.219 *	-110.499 *	11.544
600	129.013	375.71	246.70	285.18	-97.715 *	-113.105 *	9.846
700	152.151	420.54	268.39	296.30	-98.523 *	-115.617 *	8.628
800	170.746	460.71	289.96	305.21	-99.696 *	-117.983 *	7.704
900	186.122	497.11	310.99	312.60	-101.081 *	-120.170 *	6.975
1000	199.138	530.43	331.29	319.18	-100.877 *	-122.307 *	6.389
1100	210.399	561.21	350.81	325.49	-100.458 *	-124.472 *	5.911
1200	220.323	589.87	369.55	331.86	-99.820 *	-126.664 *	5.513
1300	229.220	616.76	387.54	338.52	-98.933 *	-128.936 *	5.181
1400	237.321	642.15	404.83	345.63	-97.751 *	-131.296 *	4.899
1500	244.810	666.27	421.46	353.34	-96.249 *	-133.749 *	4.658
1600	251.821	689.31	437.49	361.74	-94.354 *	-136.289 *	4.449
1700	258.466	711.42	452.95	370.92	-92.018 *	-138.988 *	4.271
1800	264.836	732.74	467.90	380.44	-89.178 *	-141.829 *	4.115

MELTING POINT	1830	K	BOILING POINT	K
ENTHALPY OF MELTING	81.000	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	33.333	kJ	MOLAR VOLUME	10.0790 J/bar 100.790 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE OXIDES				

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 5.1683 \times 10^2 - 9.2492 \times 10^{-2} T + 4.1883 \times 10^{-5} T^2 - 4.5885 \times 10^{-8} T^{0.5} - 1.4085 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K)

REFERENCE	152	227	286	COMPILED
	56		93	03-15-79

CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> GLASS

FORMULA WEIGHT 278.211

CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>: Glass 298.15 to 1500 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	237.30	237.30	210.60	-4157.300	-3942.856	690.775
UNCERTAINTY		2.50	2.50		3.300	3.320	0.581
400	58.750	304.84	246.09	247.40	-4157.923	-3869.424	505.297
500	98.874	362.62	263.75	269.91	-4156.747	-3797.422	396.716
600	128.792	413.34	284.55	286.13	-4154.675	-3725.735	324.356
700	152.209	458.43	306.22	298.85	-4152.153	-3654.446	272.700
800	171.215	499.04	327.83	309.40	-4150.181	-3583.430	233.975
900	187.089	536.02	348.93	318.49	-4147.366	-3512.734	203.875
1000	200.635	570.00	369.37	326.55	-4166.119	-3440.839	179.732
1100	212.418	601.47	389.05	333.86	-4163.105	-3368.464	159.956
1200	222.822	630.81	407.99	340.58	-4166.989	-3295.720	143.459
1300	232.123	658.33	426.21	346.85	-4161.704	-3223.338	129.516
1400	240.529	684.25	443.72	352.76	-4156.001	-3151.405	117.580
1500	248.201	708.78	460.58	358.37	-4149.877	-3079.834	107.250

MELTING POINT	1830	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	33.154	kJ	MOLAR VOLUME	10.3000 J/bar 103.000 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 720, M. P. BETA 1112, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 3.7517 \times 10^2 + 3.1970 \times 10^{-2} T - 2.4594 \times 10^{-5} T^2 + 2.8147 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	152	227	286	COMPILED
	56		148	03-15-79

CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> GLASS

FORMULA WEIGHT 278.211

CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>: Glass 298.15 to 1500 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY	FREE ENERGY	Log $K_f$
					kJ/mol	kJ/mol	
298.15	0.000	237.30	237.30	210.60	-25.111 *	-44.565 *	7.808
UNCERTAINTY		2.50	2.50		3.600	3.620	
400	58.750	304.84	246.09	247.40	-25.251 *	-51.195 *	6.685
500	98.874	362.62	263.75	269.91	-25.578 *	-57.648 *	6.023
600	128.792	413.34	284.55	286.13	-26.048 *	-64.016 *	5.573
700	152.209	458.43	306.22	298.85	-26.683 *	-70.300 *	5.246
800	171.215	499.04	327.83	309.40	-27.521 *	-76.473 *	4.993
900	187.089	536.02	348.93	318.49	-28.411 *	-82.519 *	4.790
1000	200.635	570.00	369.37	326.55	-27.580 *	-88.580 *	4.627
1100	212.418	601.47	389.05	333.86	-26.437 *	-94.737 *	4.499
1200	222.822	630.81	407.99	340.58	-25.022 *	-100.995 *	4.396
1300	232.123	658.33	426.21	346.85	-23.359 *	-107.403 *	4.315
1400	240.529	684.25	443.72	352.76	-21.461 *	-113.946 *	4.251
1500	248.201	708.78	460.58	358.37	-19.362 *	-120.627 *	4.200

MELTING POINT	1830	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	33.154	kJ	MOLAR VOLUME	10.3000 J/bar 103.000 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 3.7517 \times 10^{-2} + 3.1970 \times 10^{-5} T - 2.4594 \times 10^{-8} T^{0.5} - 2.8147 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	152	227	286	COMPILED
	56		148	03-15-79

MICROCLINE

FORMULA WEIGHT 278.333

KAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to 1400 K.

TEMP.	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	214.20	214.20	202.40	-3967.690	-3742.330	655.644
UNCERTAINTY		0.41	0.41		3.370	3.400	0.596
400	56.100	278.70	222.60	236.44	-3971.889	-3664.553	478.544
500	94.674	334.16	239.49	260.08	-3971.836	-3587.706	374.807
600	123.710	383.14	259.43	276.75	-3970.558	-3510.975	305.659
700	146.474	426.75	280.28	288.74	-3968.549	-3434.533	256.289
800	164.841	465.91	301.07	297.66	-3966.137	-3358.394	219.282
900	180.000	501.39	321.39	304.58	-3963.538	-3282.564	190.516
1000	192.749	533.78	341.03	310.27	-3971.546	-3206.286	167.480
1100	203.664	563.59	359.93	315.27	-4047.759	-3125.604	148.423
1200	213.161	591.23	378.07	319.95	-4043.555	-3041.930	132.412
1300	221.555	617.02	395.47	324.62	-4039.122	-2958.649	118.880
1400	229.093	641.25	412.16	329.50	-4034.420	-2875.727	107.295

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
$H_{298}^0 - H_0^0$	33.989 kJ	MOLAR VOLUME	10.8720 J/bar 108.720 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

- POTASSIUM.. M. P. 336.4, B. P. 1030 K.
- ALUMINUM... M. P. 933 K.
- SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 7.5955 \times 10^{-2} - 0.21711 T + 6.4333 \times 10^{-5} T^2 - 9.5268 \times 10^{-8} T^{-0.5} + 4.7642 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	90	187	93	COMPILED
	115	123	269	10- 5-76

## MICROCLINE

FORMULA WEIGHT 278.333

KAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to 1400 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	214.20	214.20	202.40	-216.154 *	-221.308 *	38.772
UNCERTAINTY		0.41	0.41		1.970	2.000	
400	56.100	278.70	222.60	236.44	-217.759 *	-222.833 *	29.099
500	94.674	334.16	239.49	260.08	-219.534 *	-223.902 *	23.391
600	123.710	383.14	259.43	276.75	-221.538 *	-224.584 *	19.552
700	146.474	426.75	280.28	288.74	-223.994 *	-224.911 *	16.783
800	164.841	465.91	301.07	297.66	-227.107 *	-224.835 *	14.680
900	180.000	501.39	321.39	304.58	-230.754 *	-224.316 *	13.019
1000	192.749	533.78	341.03	310.27	-232.315 *	-223.520 *	11.676
1100	203.664	563.59	359.93	315.27	-233.936 *	-222.569 *	10.569
1200	213.161	591.23	378.07	319.95	-235.659 *	-221.465 *	9.640
1300	221.555	617.02	395.47	324.62	-237.494 *	-220.199 *	8.848
1400	229.093	641.25	412.16	329.50	-239.409 *	-218.781 *	8.163

## MELTING POINT

K

## BOILING POINT

K

## ENTHALPY OF MELTING

kJ

## ENTHALPY OF VAPORIZATION

kJ

 $H_{298}^0 - H_0^0$ 

33.989 kJ

## MOLAR VOLUME

10.8720 J/bar  
108.720 cm<sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

K<sub>2</sub>O..... DECOMPOSES ABOVE 1154 K.SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 7.5955 \times 10^{-2} - 0.21711 T + 6.4333 \times 10^{-5} T^2 - 9.5268 \times 10^{-8} T^{-0.5} \\ + 4.7642 \times 10^{-6} T^{-2} \\ \text{(EQUATION VALID FROM 298 - 1400 K)}$$

REFERENCE	90	187	93	COMPILED
	115	123	269	10- 5-76

HIGH SILICIDE

FORMULA WEIGHT 278.333

KAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to melting point 1473 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS							
	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	S <sub>T</sub> <sup>0</sup> J/mol·K	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T J/mol·K	C <sub>P</sub> <sup>0</sup> J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>	
298.15	0.000	232.90	232.90	204.50	-3959.560	-3739.776	655.196	
UNCERTAINTY		0.48	0.48		3.370	3.400	0.596	
400	56.725	298.12	241.39	238.93	-3963.509	-3663.941	478.464	
500	95.638	354.10	258.46	262.24	-3963.224	-3589.064	374.949	
600	124.845	403.44	278.59	278.61	-3961.747	-3514.344	305.952	
700	147.699	447.32	299.62	290.43	-3959.562	-3439.945	256.693	
800	166.117	486.71	320.59	299.26	-3956.986	-3365.883	219.771	
900	181.311	522.36	341.05	306.11	-3954.228	-3292.127	191.071	
1000	194.073	554.91	360.84	311.68	-3962.092	-3217.962	168.090	
1100	204.986	584.85	379.86	316.46	-4038.174	-3139.405	149.079	
1200	214.458	612.57	398.11	320.81	-4033.868	-3057.851	133.105	
1300	222.800	638.42	415.62	324.99	-4029.373	-2976.720	119.607	
1400	230.250	662.65	432.40	329.19	-4024.670	-2895.937	108.049	

MELTING POINT	1473 K	BOILING POINT	K
ENTHALPY OF MELTING	61.500 kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	33.989 kJ	MOLAR VOLUME	10.9050 J/bar 109.050 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 6.9337 \times 10^2 - 0.17170 T + 4.9188 \times 10^{-5} T^2 - 8.3054 \times 10^{-8} T^{-0.5} + 3.4622 \times 10^4 T^{-2}$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	90	187	93	COMPILED
	115			10- 5-76

## HIGH SANIDINE

FORMULA WEIGHT 278.333

KAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to melting point 1473 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY	FREE ENERGY	Log $K_f$
					kJ/mol	kJ/mol	
298.15	0.000	232.90	232.90	204.50	-208.024 *	-218.754 *	38.325
UNCERTAINTY		0.48	0.48		1.970	2.000	
400	56.725	298.12	241.39	238.93	-209.379 *	-222.221 *	29.019
500	95.638	354.10	258.46	262.24	-210.922 *	-225.260 *	23.533
600	124.845	403.44	278.59	278.61	-212.727 *	-227.953 *	19.845
700	147.699	447.32	299.62	290.43	-215.007 *	-230.323 *	17.187
800	166.117	486.71	320.59	299.26	-217.956 *	-232.324 *	15.169
900	181.311	522.36	341.05	306.11	-221.444 *	-233.879 *	13.574
1000	194.073	554.91	360.84	311.68	-222.861 *	-235.196 *	12.285
1100	204.986	584.85	379.86	316.46	-224.351 *	-236.370 *	11.224
1200	214.458	612.57	398.11	320.81	-225.972 *	-237.386 *	10.333
1300	222.800	638.42	415.62	324.99	-227.745 *	-238.270 *	9.574
1400	230.250	662.65	432.40	329.19	-229.659 *	-238.991 *	8.917

MELTING POINT	1473 K	BOILING POINT	K
ENTHALPY OF MELTING	61.500 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	33.989 kJ	MOLAR VOLUME	10.9050 J/bar 109.050 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

K<sub>2</sub>O..... DECOMPOSES ABOVE 1154 K.SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 6.9337 \times 10^{-2} - 0.17170 T + 4.9188 \times 10^{-5} T^2 - 8.3054 \times 10^{-8} T^{-0.5} \\ + 3.4622 \times 10^{-6} T^{-2} \\ \text{(EQUATION VALID FROM 298 - 1400 K)}$$

REFERENCE	90 115	187	93	COMPILED	10- 5-76
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KAlSi<sub>3</sub>O<sub>8</sub> GLASS

FORMULA WEIGHT 278.333

KAlSi<sub>3</sub>O<sub>8</sub>: Glass 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	261.60	261.60	209.40	-3914.740	-3703.513	648.843
UNCERTAINTY		1.78	1.78		3.370	3.500	0.613
400	57.925	328.21	270.28	243.67	-3918.209	-3630.677	474.120
500	97.564	385.26	287.70	267.09	-3917.441	-3558.861	371.793
600	127.262	435.49	308.23	283.48	-3915.477	-3487.304	303.598
700	150.459	480.12	329.66	295.14	-3912.810	-3416.153	254.918
800	169.097	520.11	351.01	303.57	-3909.782	-3345.399	218.433
900	184.400	556.24	371.84	309.76	-3906.628	-3275.019	190.078
1000	197.178	589.12	391.94	314.39	-3914.167	-3204.247	167.373
1100	208.003	619.26	411.26	317.95	-3990.036	-3129.118	148.590
1200	217.286	647.05	429.76	320.77	-3985.655	-3051.014	132.808
1300	225.339	672.82	447.48	323.12	-3981.252	-2973.319	119.470

MELTING POINT	1473	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	34.884	kJ	MOLAR VOLUME	11.6500 J/bar 116.500 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_p^0 = 6.8469 \times 10^{-2} - 0.14814 T + 3.3049 \times 10^{-5} T^2 - 8.1819 \times 10^{-9} T^{-0.5} + 3.5277 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	152	227	93	COMPILED
	56		269	12- 3-76

KAlSi<sub>3</sub>O<sub>8</sub> GLASS

FORMULA WEIGHT 278.333

KAlSi<sub>3</sub>O<sub>8</sub>: Glass 298.15 to 1300 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	261.60	261.60	209.40	-163.204 *	-182.491 *	31.972
UNCERTAINTY		1.78	1.78		1.970	2.000	
400	57.925	328.21	270.28	243.67	-164.079 *	-188.957 *	24.675
500	97.564	385.26	287.70	267.09	-165.139 *	-195.057 *	20.378
600	127.262	435.49	308.23	283.48	-166.457 *	-200.913 *	17.491
700	150.459	480.12	329.66	295.14	-168.255 *	-206.531 *	15.412
800	169.097	520.11	351.01	303.57	-170.752 *	-211.840 *	13.832
900	184.400	556.24	371.84	309.76	-173.844 *	-216.771 *	12.581
1000	197.178	589.12	391.94	314.39	-174.936 *	-221.481 *	11.569
1100	208.003	619.26	411.26	317.95	-176.213 *	-226.083 *	10.736
1200	217.286	647.05	429.76	320.77	-177.759 *	-230.549 *	10.036
1300	225.339	672.82	447.48	323.12	-179.624 *	-234.869 *	9.437

MELTING POINT	1473	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	34.884	kJ	MOLAR VOLUME	11.6500 J/bar 116.500 cm <sup>3</sup>
TRANSITIONS IN REFERENCE STATE OXIDES				

K<sub>2</sub>O..... DECOMPOSES ABOVE 1154 K.SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 6.8469 \times 10^2 - 0.14814 T + 3.3049 \times 10^{-5} T^2 - 8.1819 \times 10^3 T^{-0.5} + 3.5277 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1300 K)

REFERENCE	152	227	93	COMPILED
	56		269	12- 3-76

KALIOPHILLITE

FORMULA WEIGHT 158.164

KAlSiO<sub>4</sub>: Low kaliophillite 298.15 to 810 K. High kaliophillite 810 to 1800 K.

FORMATION FROM THE ELEMENTS							
GIBBS							
TEMP.	(H <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	S <sub>T</sub> <sup>0</sup>	-(G <sub>T</sub> <sup>0</sup> -H <sub>298</sub> <sup>0</sup> )/T	C <sub>P</sub> <sup>0</sup>	ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	133.26	133.26	119.79	-2121.920	-2005.975	351.440
UNCERTAINTY		1.25	1.25		1.435	1.450	0.254
400	32.800	170.98	138.18	137.02	-2125.083	-1965.763	256.703
500	55.016	203.04	148.02	150.34	-2124.839	-1925.949	201.203
600	71.865	231.47	159.60	161.62	-2123.719	-1886.263	164.214
700	85.416	257.15	171.73	171.62	-2121.882	-1846.824	137.812
800	96.770	280.67	183.90	180.75	-2119.442	-1807.682	118.030
810	97.751	286.45	188.70	181.63	-2109.308	-1806.875	116.521
810	98.327	287.03	188.70	177.65	-2108.842	-1806.875	116.521
900	106.256	303.87	197.61	177.65	-2116.778	-1770.441	102.754
1000	113.391	322.58	209.19	177.65	-2125.596	-1731.296	90.434
1100	119.233	339.52	220.29	177.65	-2202.973	-1687.653	80.140
1200	124.101	354.97	230.87	177.65	-2200.265	-1640.911	71.427
1300	128.219	369.19	240.97	177.65	-2197.660	-1594.403	64.064
1400	131.750	382.36	250.61	177.65	-2195.148	-1548.112	57.761
1500	134.810	394.61	259.80	177.65	-2192.717	-1501.961	52.303
1600	137.487	406.08	268.59	177.65	-2190.362	-1456.006	47.534
1700	139.850	416.85	277.00	177.65	-2238.580	-1409.749	43.317
1800	141.949	427.00	285.05	177.65	-2236.068	-1361.029	39.496

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	kJ	MOLAR VOLUME	5.9890 J/bar 59.890 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. H. P. 336.4, B. P. 1030 K.

ALUMINUM... H. P. 933 K.

SILICON.... H. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 1.8888 \times 10^2 + 5.5187 \times 10^{-2} T - 1.4787 \times 10^{-5} T^2 \text{ (EQUATION VALID FROM 298 - 810 K)}$$

REFERENCE	201	120	93	CORFILED
			15	7-15-76

## KALIOPHILLITE

FORMULA WEIGHT 158.164

KAlSiO<sub>4</sub>: Low kaliophillite 298.15 to 810 K. High kaliophillite 810 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	133.26	133.26	119.79	-191.784 *	-197.529 *	34.606
UNCERTAINTY		1.25	1.25		1.605	1.620	
400	32.800	170.98	138.18	137.02	-192.649 *	-199.363 *	26.034
500	55.016	203.04	148.02	150.34	-193.617 *	-200.935 *	20.992
600	71.865	231.47	159.60	161.62	-194.493 *	-202.308 *	17.613
700	85.416	257.15	171.73	171.62	-195.231 *	-203.554 *	15.189
800	96.770	280.67	183.90	180.75	-195.834 *	-204.698 *	13.365
810	97.751	286.45	188.70	181.63	-195.928 *	-207.618 *	13.389
810	98.327	287.03	188.70	177.65	-195.462 *	-207.618 *	13.389
900	106.256	303.87	197.61	177.65	-196.514 *	-207.337 *	12.034
1000	113.391	322.58	209.19	177.65	-197.369 *	-208.494 *	10.891
1100	119.233	339.52	220.29	177.65	-198.614 *	-209.565 *	9.951
1200	124.101	354.97	230.87	177.65	-200.243 *	-210.479 *	9.162
1300	128.219	369.19	240.97	177.65	-202.248 *	-211.251 *	8.488
1400	131.750	382.36	250.61	177.65	-204.619 *	-211.865 *	7.905
1500	134.810	394.61	259.80	177.65	-207.359 *	-212.287 *	7.393
1600	137.487	406.08	268.59	177.65	-210.456 *	-212.512 *	6.938
1700	139.850	416.85	277.00	177.65	-213.910 *	-212.541 *	6.531
1800	141.949	427.00	285.05	177.65	-217.719 *	-212.347 *	6.162

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.9890 J/bar 59.890 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

K<sub>2</sub>O..... DECOMPOSES ABOVE 1154 K.SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 1.8888 \times 10^2 + 5.5187 \times 10^{-2} T - 1.4787 \times 10^3 T^{-2} \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$$

(EQUATION VALID FROM 298 - 810 K)

REFERENCE	201	120	93	COMPILED
			15	7-15-76

LEUCITE

FORMULA WEIGHT 218.248

KAlSi<sub>2</sub>O<sub>6</sub>: Tetragonal crystals 298.15 to 955 K. Cubic crystals 955 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	200.20	200.20	164.14	-3038.650	-2875.890	503.846
UNCERTAINTY		1.70	1.70		2.755	2.850	0.499
400	54.825	263.42	208.59	188.59	-3038.181	-2820.285	368.293
500	88.056	312.71	224.65	206.89	-3035.577	-2766.122	288.976
600	110.810	353.65	242.84	222.96	-3033.170	-2712.458	236.141
700	127.461	388.69	261.23	237.98	-3030.999	-2659.180	198.431
800	140.242	419.37	279.13	252.44	-3029.085	-2606.198	170.168
900	147.644	434.14	286.50	266.57	-3029.938	-2544.641	147.688
955	154.715	450.14	295.42	274.26	-3037.912	-2514.757	137.547
955	156.647	452.07	295.42	236.33	-3036.067	-2514.757	137.547
1000	160.234	462.95	302.72	236.40	-3035.252	-2490.242	130.077
1100	165.820	484.04	318.22	237.04	-3114.402	-2431.398	115.458
1200	171.800	504.71	332.91	238.18	-3111.952	-2369.394	103.138
1300	176.963	523.83	346.87	239.69	-3109.537	-2307.614	92.721
1400	181.507	541.66	360.15	241.46	-3107.109	-2246.041	83.801
1500	185.567	558.39	372.82	243.42	-3104.632	-2184.615	76.075
1600	189.249	574.16	384.91	245.53	-3102.073	-2123.364	69.321
1700	192.624	589.11	396.49	247.74	-3200.423	-2061.410	63.340
1800	195.750	603.34	407.59	250.05	-3197.060	-1994.474	57.878

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	8.8390 J/bar 88.390 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.4842 \times 10^{-2} + 0.13425 T - 2.1645 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 955 K)

$$C_P^0 = 1.9647 \times 10^{-2} + 2.7666 \times 10^{-2} T + 1.2261 \times 10^{-7} T^{-2}$$

(EQUATION VALID FROM 955 - 1800 K)

REFERENCE	201	93	93	COMPILED
		120	15	7-15-76

## LEUCITE

FORMULA WEIGHT 218.248

KAlSi<sub>3</sub>O<sub>8</sub>: Tetragonal crystals 298.15 to 955 K. Cubic crystals 955 to 1800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
					kJ/mol	kJ/mol	
298.15	0.000	200.20	200.20	164.14	-197.814 *	-211.156 *	36.994
UNCERTAINTY		1.70	1.70		2.255	2.350	
400	54.825	263.42	208.59	188.59	-194.899 *	-216.225 *	28.236
500	88.056	312.71	224.65	206.89	-193.815 *	-221.713 *	23.162
600	110.810	353.65	242.84	222.96	-194.047 *	-227.284 *	19.787
700	127.461	388.69	261.23	237.98	-195.396 *	-232.734 *	17.367
800	140.242	419.37	279.13	252.44	-197.766 *	-237.926 *	15.535
900	147.644	434.14	286.50	266.57	-203.414 *	-233.966 *	13.579
955	154.715	450.14	295.42	274.26	-202.325 *	-235.600 *	12.886
955	156.647	452.07	295.42	236.33	-200.480 *	-235.600 *	12.886
1000	160.234	462.95	302.72	236.40	-201.523 *	-237.458 *	12.404
1100	165.820	484.04	318.22	237.04	-205.311 *	-240.836 *	11.436
1200	171.800	504.71	332.91	238.18	-207.993 *	-243.946 *	10.619
1300	176.963	523.83	346.87	239.69	-211.017 *	-246.813 *	9.917
1400	181.507	541.66	360.15	241.46	-214.339 *	-249.445 *	9.307
1500	185.567	558.39	372.82	243.42	-217.953 *	-251.846 *	8.770
1600	189.249	574.16	384.91	245.53	-221.815 *	-253.952 *	8.291
1700	192.624	589.11	396.49	247.74	-225.919 *	-255.847 *	7.861
1800	195.750	603.34	407.59	250.05	-230.251 *	-257.495 *	7.472

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	8.8390 J/bar 88.390 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

K<sub>2</sub>O..... DECOMPOSES ABOVE 1154 K.SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 1.4842 \times 10^2 + 0.13425 T - 2.1645 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 955 K)

$$C_P^0 = 1.9647 \times 10^2 + 2.7666 \times 10^{-2} T + 1.2261 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 955 - 1800 K)

REFERENCE	201	93	93	COMPILED
		120	15	7-15-76

DEHYDRATED ANALCITE

FORMULA WEIGHT 202.140

NaAlSi<sub>2</sub>O<sub>6</sub>: Crystals 298.15 to 1000 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	175.40	175.40	164.40	---	---	---
UNCERTAINTY		1.70	1.70				
400	45.475	225.27	179.79	190.13	---	---	---
500	76.940	270.42	193.48	213.52	---	---	---
600	101.078	310.81	209.73	229.19	---	---	---
700	120.269	347.08	226.81	241.22	---	---	---
800	136.032	379.96	243.93	251.30	---	---	---
900	149.344	410.09	260.75	260.26	---	---	---
1000	160.854	437.94	277.09	268.51	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	J/bar

TRANSITIONS IN REFERENCE STATE ELEMENTS

- SODIUM..... M. P. 370.98, B. P. 1175 K.
- ALUMINUM... M. P. 933 K.
- SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 2.1110 \times 10^{-2} + 6.4921 \times 10^{-2} T - 7.5102 \times 10^{-4} T^2$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	201	136	COMPILED
			7-15-76

## LOW ALBITE

FORMULA WEIGHT 262.225

NaAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to 1400 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	207.40	207.40	205.10	-3935.120	-3711.722	650.281
UNCERTAINTY		0.40	0.40		3.415	3.435	0.602
400	56.950	272.87	215.92	239.71	-3939.122	-3634.926	474.675
500	95.922	328.97	233.05	262.61	-3938.777	-3558.907	371.798
600	125.125	378.36	253.23	278.80	-3937.253	-3483.046	303.227
700	147.969	422.27	274.30	290.69	-3935.004	-3407.512	254.273
800	166.396	461.70	295.30	299.69	-3932.324	-3332.333	217.580
900	181.611	497.42	315.81	306.71	-3929.418	-3257.489	189.061
1000	194.412	530.04	335.63	312.34	-3937.083	-3182.243	166.224
1100	205.350	560.03	354.68	316.99	-3933.728	-3106.923	147.536
1200	214.822	587.79	372.97	320.95	-4027.646	-3029.831	131.886
1300	223.122	613.62	390.50	324.45	-4023.167	-2946.882	118.408
1400	230.479	637.78	407.30	327.64	-4018.563	-2864.289	106.868

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	33.452 kJ	MOLAR VOLUME	10.0070 J/bar 100.070 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 5.8394 \times 10^2 - 0.092852 T + 2.2722 \times 10^{-5} T^2 - 6.4242 \times 10^3 T^{-0.5} \\ + 1.6780 \times 10^6 T^{-2} \\ \text{(EQUATION VALID FROM 298 - 1500 K)}$$

REFERENCE	115	187	93	COMPILED
	90	123		10-5-76



LOW ALBITE

FORMULA WEIGHT 262.225

NaAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to 1400 K.

TEMP.	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol
298.15	0.000	207.40	207.40	205.10	-157.760 *	-163.699 *	28.680
UNCERTAINTY		0.40	0.40		2.105	2.125	
400	56.950	272.87	215.92	239.71	-158.300 *	-165.656 *	21.633
500	95.922	328.97	233.05	262.61	-159.117 *	-167.407 *	17.489
600	125.125	378.36	253.23	278.80	-160.244 *	-168.956 *	14.709
700	147.969	422.27	274.30	290.69	-161.840 *	-170.293 *	12.707
800	166.396	461.70	295.30	299.69	-164.054 *	-171.362 *	11.189
900	181.611	497.42	315.81	306.71	-166.735 *	-172.091 *	9.988
1000	194.412	530.04	335.63	312.34	-167.241 *	-172.671 *	9.019
1100	205.350	560.03	354.68	316.99	---	---	---
1200	214.822	587.79	372.97	320.95	---	---	---
1300	223.122	613.62	390.50	324.45	---	---	---
1400	230.479	637.78	407.30	327.64	---	---	---

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	33.452 kJ	MOLAR VOLUME	10.0070 J/bar 100.070 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

- Na<sub>2</sub>O..... M. P. 1193 K.
- SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 5.8394 \times 10^{-2} - 0.092852 T + 2.2722 \times 10^{-5} T^2 - 6.4242 \times 10^{-8} T^{-0.5} + 1.6780 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1500 K)

REFERENCE	115	187	93	COMPILED
	90	123		10- 5-76

ANALBITE FORMULA WEIGHT 262.225NaAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to 1400 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_p^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	226.40	226.40	204.80	-3924.240	-3706.507	649.367
UNCERTAINTY		0.40	0.40		3.640	3.660	0.641
400	56.875	291.78	234.90	239.70	-3928.272	-3631.640	474.246
500	95.932	347.96	252.03	263.27	-3927.892	-3557.517	371.653
600	125.278	397.50	272.22	279.81	-3926.281	-3483.558	303.272
700	148.247	441.58	293.33	291.70	-3923.929	-3409.954	254.455
800	166.754	481.13	314.38	300.47	-3921.158	-3336.711	217.866
900	181.989	516.92	334.93	307.10	-3918.198	-3263.819	189.428
1000	194.773	549.55	354.78	312.27	-3925.842	-3190.512	166.656
1100	205.651	579.52	373.87	316.47	-3922.517	-3117.151	148.022
1200	215.037	607.21	392.17	320.03	-4016.508	-3041.997	132.615
1300	223.236	632.95	409.71	323.21	-4012.139	-2960.983	118.974
1400	230.486	657.01	426.52	326.20	-4007.673	-2880.321	107.467

MELTING POINT	1391	K	BOILING POINT	K
ENTHALPY OF MELTING	59.280	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	33.423	kJ	MOLAR VOLUME	10.0430 J/bar 100.430 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 6.7137 \times 10^2 - 0.14671 T + 3.6586 \times 10^{-5} T^2 - 7.9736 \times 10^3 T^{-0.5} + 3.1740 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	90	76	93	COMPILED
		187	100	10- 5-76

ANALBITE

FORMULA WEIGHT 262.225

NaAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to 1400 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY	FREE ENERGY	Log K <sub>f</sub>
					kJ/mol	kJ/mol	
298.15	0.000	226.40	226.40	204.80	-146.880 *	-158.484 *	27.766
UNCERTAINTY		0.40	0.40		2.450	2.470	
400	56.875	291.78	234.90	239.70	-147.450 *	-162.370 *	21.203
500	95.932	347.96	252.03	263.27	-148.232 *	-166.017 *	17.344
600	125.278	397.50	272.22	279.81	-149.272 *	-169.468 *	14.754
700	148.247	441.58	293.33	291.70	-150.765 *	-172.735 *	12.890
800	166.754	481.13	314.38	300.47	-152.888 *	-175.740 *	11.475
900	181.989	516.92	334.93	307.10	-155.515 *	-178.421 *	10.355
1000	194.773	549.55	354.78	312.27	-156.000 *	-180.940 *	9.451
1100	205.651	579.52	373.87	316.47	---	---	---
1200	215.037	607.21	392.17	320.03	---	---	---
1300	223.236	632.95	409.71	323.21	---	---	---
1400	230.486	657.01	426.52	326.20	---	---	---

MELTING POINT	1391 K	BOILING POINT	K
ENTHALPY OF MELTING	59.280 kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	33.423 kJ	MOLAR VOLUME	10.0430 J/bar 100.430 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

- Na<sub>2</sub>O..... H. P. 1193 K.
- SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 6.7137 \times 10^{-2} - 0.14671 T + 3.6586 \times 10^{-5} T^2 - 7.9736 \times 10^{-8} T^{-0.5} + 3.1740 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1400 K)

REFERENCE	90	76	93	COMPILED
		187	100	10- 5-76

NaAlSi<sub>3</sub>O<sub>8</sub> GLASS

FORMULA WEIGHT 262.225

NaAlSi<sub>3</sub>O<sub>8</sub>: Glass 298.15 to 1200 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_p^0$	ENTHALPY	FREE ENERGY	Log $K_f$
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	251.90	251.90	209.90	-3875.460	-3665.330	642.153
UNCERTAINTY		1.50	1.50		3.700	3.720	0.652
400	58.325	318.96	260.63	246.01	-3878.912	-3593.152	469.220
500	98.416	376.60	278.18	269.92	-3877.870	-3521.815	367.923
600	128.448	427.35	298.90	286.29	-3875.599	-3450.786	300.419
700	151.887	472.42	320.53	298.18	-3872.601	-3380.214	252.236
800	170.782	512.87	342.09	307.62	-3869.155	-3310.100	216.128
900	186.456	549.60	363.14	315.98	-3865.398	-3240.431	188.071
1000	199.821	583.31	383.49	324.20	-3872.014	-3170.444	165.608
1100	211.520	614.62	403.10	332.94	-3867.281	-3100.525	147.232
1200	222.036	643.99	421.95	342.67	-3959.329	-3028.954	131.847

MELTING POINT	1391	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	34.257	kJ	MOLAR VOLUME	11.0086 J/bar 110.086 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

## HEAT CAPACITY EQUATION

$$C_p^0 = 9.1795 \times 10^2 - 0.38242 T + 1.4740 \times 10^{-4} T^2 - 1.1511 \times 10^{-6} T^{-0.5} \\ + 5.2796 \times 10^{-6} T^{-2} \\ \text{(EQUATION VALID FROM 298 - 1200 K)}$$

REFERENCE	152	227	93 269	COMPILED 10-19-76
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NaAlSi<sub>3</sub>O<sub>8</sub> GLASS

FORMULA WEIGHT 262.225

NaAlSi<sub>3</sub>O<sub>8</sub>: Glass 298.15 to 1200 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	251.90	251.90	209.90	-98.100 *	-117.307 *	20.552
UNCERTAINTY		1.50	1.50		2.510	2.530	
400	58.325	318.96	260.63	246.01	-98.090 *	-123.882 *	16.177
500	98.416	376.60	278.18	269.92	-98.210 *	-130.315 *	13.614
600	128.448	427.35	298.90	286.29	-98.590 *	-136.696 *	11.901
700	151.887	472.42	320.53	298.18	-99.437 *	-142.995 *	10.670
800	170.782	512.87	342.09	307.62	-100.885 *	-149.129 *	9.737
900	186.456	549.60	363.14	315.98	-102.715 *	-155.033 *	8.998
1000	199.821	583.31	383.49	324.20	-102.172 *	-160.872 *	8.403
1100	211.520	614.62	403.10	332.94	---	---	---
1200	222.036	643.99	421.95	342.67	---	---	---

MELTING POINT	1391	K	BOILING POINT	K
ENTHALPY OF MELTING		KJ	ENTHALPY OF VAPORIZATION	KJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	34.257	KJ	MOLAR VOLUME	11.0086 J/bar 110.086 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

Na<sub>2</sub>O..... M. P. 1193 K.

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 9.1795 \times 10^2 - 0.38242 T + 1.4740 \times 10^{-4} T^2 - 1.1511 \times 10^{-6} T^{0.5} + 5.2796 \times 10^{-8} T^3$$

(EQUATION VALID FROM 298 - 1200 K)

REFERENCE	152	227	93	COMPILED
			269	10-19-76

## NEPHELINE

FORMULA WEIGHT 142.055

NaAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to 1521 K. Carnegieite is the stable phase above  
1521 K. α - β transition at 467 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	124.35	124.35	115.81	-2092.110	-1977.498	346.449
UNCERTAINTY		1.25	1.25		2.420	2.450	0.429
400	32.372	161.59	129.22	145.90	-2095.587	-1937.982	253.076
500	52.552	196.36	143.81	145.64	-2096.396	-1901.019	198.599
600	72.662	223.80	151.14	152.36	-2093.545	-1859.733	161.905
700	84.577	247.82	163.24	159.07	-2092.730	-1820.801	135.870
800	94.140	269.33	175.19	165.78	-2091.737	-1782.022	116.355
900	102.136	288.91	186.77	172.49	-2090.576	-1743.390	101.184
1000	108.993	306.86	197.86	179.20	-2099.954	-1704.090	89.013
1100	115.516	324.09	208.58	185.91	-2097.645	-1664.623	79.047
1180	120.471	337.48	217.01	191.28	-2192.761	-1632.754	72.276
1180	121.244	338.25	217.01	178.51	-2191.807	-1632.754	72.276
1200	122.207	341.12	218.92	178.62	-2191.381	-1623.349	70.663
1300	126.582	355.47	228.89	179.18	-2188.631	-1576.151	63.331
1400	130.361	368.78	238.42	179.73	-2185.935	-1529.162	57.054
1500	133.665	381.20	247.54	180.28	-2183.278	-1482.351	51.620

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	5.4160 J/bar 54.160 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

SODIUM..... M. P. 370.98, B. P. 1175 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

## HEAT CAPACITY EQUATIONS

$$C_P^0 = 27.74 + 0.2954 T$$

(EQUATION VALID FROM 298 - 467 K)

$$C_P^0 = 112.09 + 0.06711 T$$

(EQUATION VALID FROM 467 - 1180 K)

$$C_P^0 = 172.00 + 0.00552 T$$

(EQUATION VALID FROM 1180 - 1525 K)

REFERENCE	115	120	93	COMPILED
			229	4-15-76

NEPHELINE

FORMULA WEIGHT 142.055

NaAlSi<sub>3</sub>O<sub>8</sub>: Crystals 298.15 to 1521 K. Carnegieite is the stable phase above 1521 K.

TEMP.	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	124.35	124.35	115.81	-136.150 *	-142.052 *	24.887
UNCERTAINTY		1.25	1.25				
400	32.372	161.59	129.22	145.90	-136.461 *	-144.032 *	18.809
500	52.552	196.36	143.81	145.64	-137.816 *	-148.309 *	15.494
600	72.662	223.80	151.14	152.36	-136.330 *	-148.080 *	12.892
700	84.577	247.82	163.24	159.07	-137.470 *	-149.934 *	11.188
800	94.140	269.33	175.19	165.78	-138.889 *	-151.626 *	9.900
900	102.136	288.91	186.77	172.49	-140.413 *	-153.136 *	8.888
1000	108.993	306.86	197.86	179.20	-141.116 *	-154.482 *	8.069
1100	115.516	324.09	208.58	185.91	---	---	---
1180	120.471	337.48	217.01	191.28	---	---	---
1180	121.244	338.25	217.01	178.51	---	---	---
1200	122.207	341.12	218.92	178.62	---	---	---
1300	126.582	355.47	228.89	179.18	---	---	---
1400	130.361	368.78	238.42	179.73	---	---	---
1500	133.665	381.20	247.54	180.28	---	---	---

MELTING POINT

K

BOILING POINT

K

ENTHALPY OF MELTING

kJ

ENTHALPY OF VAPORIZATION

kJ

$H_{298}^0 - H_0^0$

kJ

MOLAR VOLUME

5.4160 J/bar  
54.160 cm<sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

Na<sub>2</sub>O..... M. P. 1193 K.

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

REFERENCE 115

120

93

COMPILED

229

4-15-76

## MUSCOVITE

FORMULA WEIGHT 398.311

KAl<sub>2</sub>[AlSi<sub>3</sub>O<sub>10</sub>](OH)<sub>2</sub>: Crystals 298.15 to 1500 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	306.40	306.40	326.10	-5976.740	-5600.671	981.219
UNCERTAINTY		0.61	0.61		3.235	3.290	0.576
400	91.100	411.12	320.02	385.54	-5981.048	-5471.333	714.486
500	154.242	501.73	347.49	425.67	-5979.503	-5344.043	558.291
600	202.007	582.02	380.01	454.42	-5975.746	-5217.261	454.205
700	239.653	653.74	414.09	475.56	-5970.644	-5091.248	379.915
800	270.176	718.32	448.14	491.35	-5964.809	-4965.994	324.248
900	295.444	776.92	481.48	503.24	-5958.697	-4841.485	280.994
1000	316.693	830.42	513.73	512.16	-5984.613	-4715.393	246.308

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	49.443 kJ	MOLAR VOLUME	14.0710 J/bar 140.710 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 9.1767 \times 10^{-2} - 8.1110 \times 10^{-5} T - 1.0348 \times 10^{-8} T^{-0.5} + 2.8341 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	152	226	93	COMPILED
	199	277	12	10-22-76



MUSCOVITE

FORMULA WEIGHT 398.311

KAl<sub>2</sub>[AlSi<sub>2</sub>O<sub>10</sub>](OH)<sub>2</sub>: Crystals 298.15 to 1500 K.

TEMP. K	(H <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	S <sub>T</sub> <sup>o</sup> J/mol·K	-(G <sub>T</sub> <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T J/mol·K	C <sub>p</sub> <sup>o</sup> J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	306.40	306.40	326.10	-263.674 *	-260.280 *	45.600
UNCERTAINTY						2.525	2.550
400	91.100	411.12	320.02	385.54	-307.778 *	-255.569 *	33.374
500	154.242	501.73	347.49	425.67	-307.397 *	-242.550 *	25.339
600	202.007	582.02	380.01	454.42	-306.704 *	-229.625 *	19.991
700	239.653	653.74	414.09	475.56	-306.050 *	-216.849 *	16.182
800	270.176	718.32	448.14	491.35	-305.769 *	-204.121 *	13.329
900	295.444	776.92	481.48	503.24	-305.863 *	-191.398 *	11.109
1000	316.693	830.42	513.73	512.16	-303.825 *	-178.780 *	9.339

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	KJ	ENTHALPY OF VAPORIZATION	KJ
H <sub>298</sub> <sup>o</sup> - H <sub>0</sub> <sup>o</sup>	49.443 kJ	MOLAR VOLUME	14.0710 J/bar 140.710 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE OXIDES

- K<sub>2</sub>O..... DECOMPOSES ABOVE 1154 K.
- SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.
- H<sub>2</sub>O..... B. P. 373.15 K.

HEAT CAPACITY EQUATION

$$C_p^o = 9.1767 \times 10^{-2} - 8.1110 \times 10^{-2} T - 1.0348 \times 10^{-4} T^{-0.5} + 2.8341 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 1000 K)

REFERENCE	152	226	93	COMPILED
	199	277	12	10-22-76

## FLUORPHLOGOPITE

FORMULA WEIGHT 421.244

=====  
 KMg<sub>3</sub>(AlSi<sub>3</sub>O<sub>10</sub>)F<sub>2</sub>: Crystals 298.15 to melting point 1670 K. Liquid 1670 to  
 1800 K.  
 =====

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	336.30	336.30	342.40	-6392.880	-6053.067	1060.477
UNCERTAINTY		2.10	2.10		3.660	3.800	0.666
-----							
400	94.325	444.81	350.48	392.83	-6395.894	-5936.351	775.211
500	157.048	535.72	378.67	420.87	-6394.402	-5821.622	608.183
600	202.693	614.23	411.54	439.96	-6391.926	-5707.271	496.864
700	237.664	683.18	445.52	454.48	-6388.999	-5593.399	417.386
800	265.530	744.67	479.14	466.38	-6385.882	-5479.948	357.805
900	288.433	800.21	511.78	476.62	-6382.729	-5366.855	311.486
-----							
1000	307.712	850.90	543.19	485.76	-6417.149	-5251.119	274.292
-----							
1100	324.284	897.60	573.32	494.13	-6492.677	-5130.390	243.623
1200	338.765	940.93	602.16	501.92	-6487.537	-5006.741	217.939
1300	351.602	981.40	629.80	509.29	-6481.933	-4883.581	196.226
-----							
1400	363.114	1019.40	656.29	516.32	-6856.764	-4750.073	177.228
1500	373.557	1055.26	681.70	523.09	-6846.697	-4599.943	160.185
1600	383.109	1089.22	706.11	529.64	-6836.183	-4450.468	145.293

MELTING POINT	1670	K	BOILING POINT	K
ENTHALPY OF MELTING	308.779	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$		kJ	MOLAR VOLUME	14.6370 J/bar 146.370 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE ELEMENTS

POTASSIUM.. M. P. 336.4, B. P. 1030 K.

MAGNESIUM.. M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

ALUMINUM... M. P. 933 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 4.9287 \times 10^2 + 4.9103 \times 10^{-2} T - 1.5688 \times 10^{-5} T^2 - 6.5987 \times 10^{-9} T^3$$

(EQUATION VALID FROM 298 - 1670 K)

REFERENCE	118	118	93	COMPILED
		257	118	8-26-76

TALC

FORMULA WEIGHT 379.268

Hg<sub>3</sub>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>: Crystals 298.15 to 1100 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	260.83	260.83	321.70	-5915.900	-5536.048	969.897
UNCERTAINTY		0.63	0.63		4.330	4.350	0.762
400	90.925	365.30	274.38	386.59	-5917.050	-5405.971	705.950
500	153.808	455.61	301.80	420.63	-5914.990	-5278.425	551.436
600	200.257	534.40	334.14	444.26	-5911.596	-5151.383	448.470
700	237.119	604.91	367.79	475.20	-5906.844	-5024.997	374.972
800	270.051	669.80	399.75	525.95	-5898.951	-4898.009	319.809

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H <sub>298</sub> <sup>0</sup> - H <sub>0</sub> <sup>0</sup>	46.886 kJ	MOLAR VOLUME	13.6250 J/bar 136.250 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 5.6536 \times 10^{-3} - 5.2717 T + 2.7291 \times 10^{-3} T^2 - 7.6926 \times 10^{-6} T^{-0.5} + 4.0211 \times 10^7 T^{-2}$$

(EQUATION VALID FROM 298 - 800 K)

REFERENCE	151	228	93	COMPILED
	28		11	8-26-76

TALC

FORMULA WEIGHT 379.268

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 $\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$ : Crystals 298.15 to 1100 K.  
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TEMP. K	FORMATION FROM THE OXIDES				GIBBS		
	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	260.83	260.83	321.70	-182.800 *	-166.167 *	29.112
UNCERTAINTY		0.63	0.63		1.420	1.450	
400	90.925	365.30	274.38	386.59	-226.319 *	-157.007 *	20.503
500	153.808	455.61	301.80	420.63	-225.104 *	-139.799 *	14.605
600	200.257	534.40	334.14	444.26	-224.147 *	-122.829 *	10.693
700	237.119	604.91	367.79	475.20	-223.114 *	-105.961 *	7.907
800	270.051	669.80	399.75	525.95	-220.077 *	-87.917 *	5.740

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	46.886 kJ	MOLAR VOLUME	13.6250 J/bar 136.250 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.

H<sub>2</sub>O..... B. P. 373.15 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 5.6536 \times 10^{-3} - 5.2717 T + 2.7291 \times 10^{-3} T^2 - 7.6926 \times 10^{-6} T^{-0.5} \\ + 4.0211 \times 10^7 T^{-2} \\ \text{(EQUATION VALID FROM 298 - 800 K)}$$

REFERENCE	151	228	93	COMPILED
	28		11	8-26-76

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PHYROPHYLLITE

FORMULA WEIGHT 360.317

$Al_2Si_4O_{10}(OH)_2$ : Crystals 298.15 to 800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log $K_f$
298.15	0.000	239.40	239.40	293.70	-5639.800	-5265.884	922.565
UNCERTAINTY		0.40	0.40		3.950	3.960	0.694
400	82.450	334.16	251.71	349.62	-5641.641	-5137.750	670.924
500	139.748	416.33	276.58	386.06	-5640.439	-5011.889	523.590
600	183.103	489.17	306.07	412.41	-5637.406	-4886.421	425.402
700	217.363	554.32	336.96	432.59	-5633.192	-4761.587	355.316
800	245.309	613.17	367.86	448.71	-5628.207	-4637.392	302.791

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	42.695 kJ	MOLAR VOLUME	12.7820 J/bar 127.820 $cm^3$

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 7.4675 \times 10^{-2} - 5.3543 \times 10^{-2} T + 1.9855 \times 10^{-5} T^2 - 7.5777 \times 10^{-9} T^{-0.5}$$

(EQUATION VALID FROM 298 - 800 K)

REFERENCE	152	226	286	COMPILED
		139	152	03-15-79

## PYROPHYLLITE

FORMULA WEIGHT 360.317

Al<sub>2</sub>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>: Crystals 298.15 to 800 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	239.40	239.40	293.70	-35.470 *	-21.363 *	3.743
UNCERTAINTY		0.40	0.40		1.325	1.350	
400	82.450	334.16	251.71	349.62	-79.109 *	-13.065 *	1.706
500	139.748	416.33	276.58	386.06	-78.475 *	3.380 *	-0.366
600	183.103	489.17	306.07	412.41	-77.796 *	19.697 *	-1.715
700	217.363	554.32	336.96	432.59	-77.346 *	35.894 *	-2.678
800	245.309	613.17	367.86	448.71	-77.354 *	52.071 *	-3.400

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	42.695 kJ	MOLAR VOLUME	12.5900 J/bar 125.900 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.H<sub>2</sub>O..... B. P. 373.15 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 7.4675 \times 10^{-2} - 5.3543 \times 10^{-2} T + 1.9855 \times 10^{-5} T^2 - 7.5777 \times 10^{-9} T^{-0.5}$$

(EQUATION VALID FROM 298 - 800 K)

REFERENCE	152	226	286	COMPILED
		139	152	03-15-79

CHRYSOITILE

FORMULA WEIGHT 277.113

Mg<sub>3</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub>: Crystals 298.15 to 900 K.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^0 - H_{298}^0)/T$	$S_T^0$	$-(G_T^0 - H_{298}^0)/T$	$C_P^0$	ENTHALPY	GIBBS FREE ENERGY	Log $K_f$
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	221.30	221.30	273.70	-4361.660	-4034.024	706.747
UNCERTAINTY		0.80	0.80		3.480	3.500	0.613
400	76.425	309.13	232.70	323.22	-4362.729	-3921.820	512.139
500	129.292	385.05	255.76	356.33	-4360.883	-3811.788	398.216
600	169.133	452.14	283.01	378.95	-4357.294	-3702.258	322.312
700	200.273	511.78	311.51	394.26	-4352.759	-3593.454	268.148
800	225.195	565.13	339.93	404.32	-4347.832	-3485.318	227.569
900	245.467	613.14	367.67	410.47	-4342.911	-3377.752	196.041

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	10.8500 J/bar 108.500 cm <sup>3</sup>

TRANSITIONS IN REFERENCE STATE ELEMENTS

MAGNESIUM.. M. P. 922, B. P. 1361 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION

$$C_P^0 = 8.9960 \times 10^{-2} - 0.14476 T - 1.0932 \times 10^{-6} T^{-0.5} + 4.4999 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	128	128	93	COMPILED
			128	9- 3-76

## CHRYSTOTILE

FORMULA WEIGHT 277.113

Mg<sub>3</sub>Si<sub>2</sub>O<sub>8</sub>(OH)<sub>4</sub>: Crystals 298.15 to 900 K.

TEMP. K	$(H_T^0 - H_{298}^0)/T$ J/mol·K	$S_T^0$ J/mol·K	$-(G_T^0 - H_{298}^0)/T$ J/mol·K	$C_P^0$ J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	Log K <sub>f</sub>
298.15	0.000	221.30	221.30	273.70	-164.130 *	-139.578 *	24.454
UNCERTAINTY		0.80	0.80		2.710	2.750	
400	76.425	309.13	232.70	323.22	-250.858 *	-124.294 *	16.231
500	129.292	385.05	255.76	356.33	-248.257 *	-92.917 *	9.707
600	169.133	452.14	283.01	378.95	-244.891 *	-62.154 *	5.411
700	200.273	511.78	311.51	394.26	-241.301 *	-31.985 *	2.387
800	225.195	565.13	339.93	404.32	-237.938 *	-2.327 *	0.152
900	245.467	613.14	367.67	410.47	-234.968 *	26.957 *	-1.565

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^0 - H_0^0$	kJ	MOLAR VOLUME	10.8500 J/bar 108.500 cm <sup>3</sup>

## TRANSITIONS IN REFERENCE STATE OXIDES

SiO<sub>2</sub>..... ALPHA - BETA TRANSITION 844 K.H<sub>2</sub>O..... B. P. 373.15 K.

## HEAT CAPACITY EQUATION

$$C_P^0 = 8.9960 \times 10^{-4} T^2 - 0.14476 T - 1.0932 \times 10^4 T^{-0.5} + 4.4999 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 298 - 900 K)

REFERENCE	128	128	93	COMPILED
			128	9- 3-76





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